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* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 AUG 09 INSPEC enhanced with 1898-1968 archive
NEWS 4 AUG 28 ADISCTI Reloaded and Enhanced
NEWS 5 AUG 30 CA(SM)/Cplus(SM) Austrian patent law changes
NEWS 6 SEP 21 CA/Cplus fields enhanced with simultaneous left and right
truncation
NEWS 7 SEP 25 CA(SM)/Cplus(SM) display of CA Lexicon enhanced
NEWS 8 SEP 25 CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS 9 SEP 25 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 10 SEP 28 CEABA-VTB classification code fields reloaded with new
classification scheme
NEWS 11 OCT 19 LOGOFF HOLD duration extended to 120 minutes
NEWS 12 OCT 19 E-mail format enhanced
NEWS 13 OCT 23 Option to turn off MARPAT highlighting enhancements available
NEWS 14 OCT 23 CAS Registry Number crossover limit increased to 300,000 in
multiple databases
NEWS 15 OCT 23 The Derwent World Patents Index suite of databases on STN
has been enhanced and reloaded
NEWS 16 OCT 30 CHEMLIST enhanced with new search and display field
NEWS 17 NOV 03 JAPIO enhanced with IPC 8 features and functionality
NEWS 18 NOV 10 CA/Cplus F-Term thesaurus enhanced
NEWS 19 NOV 10 STN Express with Discover! free maintenance release Version
8.01c now available
NEWS 20 NOV 20 CAS Registry Number crossover limit increased to 300,000 in
additional databases
NEWS 21 NOV 20 CA/Cplus to MARPAT accession number crossover limit increased
to 50,000
NEWS 22 DEC 01 CAS REGISTRY updated with new ambiguity codes
NEWS 23 DEC 11 CAS REGISTRY chemical nomenclature enhanced
NEWS 24 DEC 14 WPIDS/WPINDEX/WPIX manual codes updated
NEWS 25 DEC 14 GBFULL and FRFULL enhanced with IPC 8 features and
functionality
NEWS 26 DEC 18 CA/Cplus pre-1967 chemical substance index entries enhanced
with preparation role
NEWS 27 DEC 18 CA/Cplus patent kind codes updated
NEWS 28 DEC 18 MARPAT to CA/Cplus accession number crossover limit increased
to 50,000
NEWS 29 DEC 18 MEDLINE updated in preparation for 2007 reload
NEWS 30 DEC 27 CA/Cplus enhanced with more pre-1907 records

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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NEWS IPC8 For general information regarding STN implementation of IPC 8
NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 07:49:52 ON 08 JAN 2007

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 07:50:03 ON 08 JAN 2007

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 JAN 2007 HIGHEST RN 916885-50-2

DICTIONARY FILE UPDATES: 7 JAN 2007 HIGHEST RN 916885-50-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

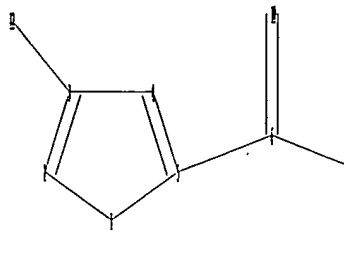
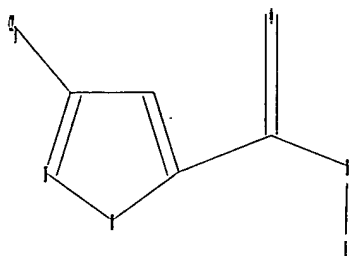
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10519356\Struc 4.str



```

chain nodes :
6 7 10 11 12
ring nodes :
1 2 3 4 5
chain bonds :
3-12 5-6 6-7 6-10 7-11
ring bonds :
1-5 1-2 2-3 3-4 4-5
exact/norm bonds :
1-5 1-2 2-3 3-4 4-5 6-7 6-10
exact bonds :
3-12 5-6 7-11

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G1:Cb,Cy,Hy

G2:S,N

Match level :

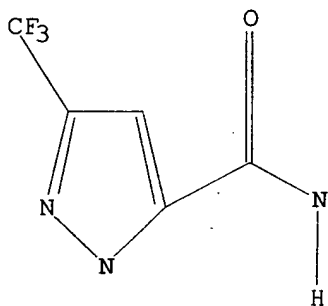
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 10:CLASS 11:CLASS
12:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 Cb,Cy,Hy

G2 S,N

Structure attributes must be viewed using STN Express query preparation.

10519356a.trn

=> l1

SAMPLE SEARCH INITIATED 07:50:14 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 165 TO ITERATE

100.0% PROCESSED 165 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

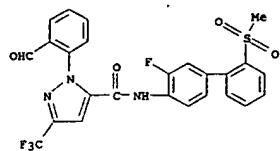
PROJECTED ITERATIONS: 2530 TO 4070

PROJECTED ANSWERS: 1761 TO 3079

L2 50 SEA SSS SAM L1

=> d scan

L2 50 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-[methylsulfonyl][1,1'-biphenyl]-
 4-yl]-1-(2-formylphenyl)-3-(trifluoromethyl)- (9CI)
 MF C25 H17 F4 N3 O4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

Page 6

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.45

0.66

FILE 'CAPLUS' ENTERED AT 07:50:41 ON 08 JAN 2007

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FILE COVERS 1907 - 8 Jan 2007 VOL 146 ISS 3

FILE LAST UPDATED: 7 Jan 2007 (20070107/ED)

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<http://www.cas.org/infopolicy.html>

=> l2

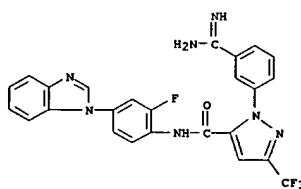
L3

28 L2

=> d ibib abs hitstr 20-28

L3 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:791919 CAPLUS
 DOCUMENT NUMBER: 141:342889
 TITLE: SAR and factor IXa crystal structure of a dual inhibitor of factors IXa and Xa
 AUTHOR(S): Smallheer, Joanne M.; Alexander, Richard S.; Wang, Jianmin; Wang, Shuaige; Nakajima, Suanne; Rossi, Karen
 Debra; A.; Smallwood, Angela; Barbera, Frank; Burdick, Luetzgen, Joseph M.; Knabb, Robert M.; Wexler, Ruth R.; Jadhav, Prabhakar K.
 CORPORATE SOURCE: Bristol-Myers Squibb Company, Princeton, NJ, 08543-5400, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(21), 5263-5267
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:342889
 AB Modifications to the P4 moiety and pyrazole C3 substituent of factor Xa inhibitor SN-429 provided several new compds., which are 5-10 nM inhibitors of factor IXa. An x-ray crystal structure of one example complexed to factor IXa shows that these compds. adopt a similar binding mode to that previously observed with pyrazole inhibitors in the factor Xa active site both with regard to how the inhibitor binds and the position of Tyr99.
 IT 848393-63-5P
 RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 of (pyrazole compds. preparation, crystal structure, and dual inhibition factors IXa and Xa)
 RN 848393-63-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)
 CM 1
 CRN 774218-46-1
 CMF C25 H17 F4 N7 O

L3 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2
 CRN 76-05-1
 CMF C2 H F3 O2



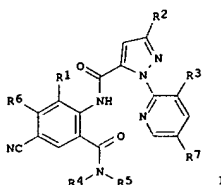
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L3 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:648522 CAPLUS
 DOCUMENT NUMBER: 141:190786
 TITLE: Preparation of cyano anthranilamide insecticides
 INVENTOR(S): Hughes, Kenneth Andrew; Lahm, George Philip; Selby, Thomas Paul; Stevenson, Thomas Martin
 PATENT ASSIGNEE(S): E.I. Du Pont De Nemours and Company, USA
 SOURCE: PCT Int. Appl., 63 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

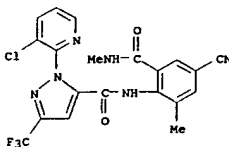
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004067528	A1	20040812	WO 2004-US3568	20040121
WO 2004067528	B1	20041007		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
AU 2004207848	A1	20040812	AU 2004-207848	20040121
CA 2512242	A1	20040812	CA 2004-2512242	20040121
EP 1599463	A1	20051130	EP 2004-704148	20040121
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
MD 2005000219	A	20051130	MD 2005-219	20040121
BR 2004006709	A	20051220	BR 2004-6709	20040121
JP 3764895	B1	20060412	JP 2005-518229	20040121
JP 2006515602	T	20060601		
CN 1829707	A	20060906	CN 2004-80002991	20040121
EG 23536	A	20060419	EG 2004-49	20040127
JP 2006028159	A	20060202	JP 2005-148184	20050520
JP 3770500	B2	20060426		
JP 2006290862	A	20061026	JP 2005-148201	20050520
US 2006111403	A1	20060525	US 2005-540966	20050629
PRIORITY APPLN. INFO.:			US 2003-443256P	P 20030128
			JP 2005-518229	A3 20040121
			WO 2004-US3568	W 20040121

OTHER SOURCE(S): MARPAT 141:190786
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L3 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

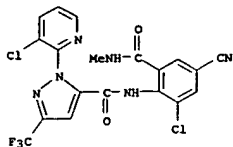


AB The title compds. I; R1 = Me, Cl, Br, F; R2 = F, Cl, Br, haloalkyl or haloalkoxy; R3 = F, Cl, Br; R4 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, each optionally substituted with one substituent selected from the group consisting of halo, CN, SMe S(O)Me, S(O)2Me and OMe; R5 = H, Me; R6 = H, F, Cl; R7 = H, F, Cl, useful for controlling an invertebrate pest, were prepared E.g., a multi-step synthesis of compound I
 (R1 = Me; R2 = CF3; R3 = Cl; R4, R5 = H), was given. The compds. I were tested in various biol. tests (data given). This invention also pertains to a composition for controlling an invertebrate pest comprising a biol. effective amount of a compound I, an N-oxide thereof or a suitable salt of the compound I and at least one addnl. component selected from the group consisting of a surfactant, a solid diluent and a liquid diluent.
 IT 736994-60-8P 736994-79-9P 736994-94-8P 736995-07-6P 736995-09-8P
 RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of cyano anthranilamide insecticides)
 RN 736994-60-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-[4-cyano-2-methyl-6-((methylamino)carbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



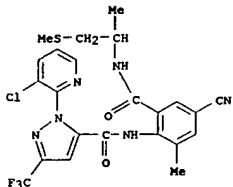
RN 736994-79-9 CAPLUS

L3 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CN 1H-Pyrazole-5-carboxamide, N-[2-chloro-4-cyano-6-
 [(methylamino)carbonyl]phenyl]-1-(3-chloro-2-pyridinyl)-3-
 (trifluoromethyl)- (9CI) (CA INDEX NAME)



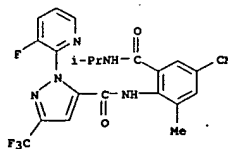
RN 736994-94-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 1-(3-chloro-2-pyridinyl)-N-[4-cyano-2-methyl-6-

[[1-methyl-2-(methylthio)ethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)-
 (9CI) (CA INDEX NAME)

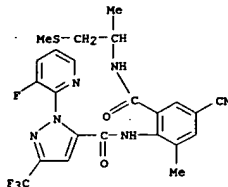


RN 736995-07-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[4-cyano-2-methyl-6-[[1-
 methylethyl]amino]carbonyl]phenyl]-1-(3-fluoro-2-pyridinyl)-3-
 (trifluoromethyl)- (9CI) (CA INDEX NAME)

L3 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 736995-09-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[4-cyano-2-methyl-6-[[1-methyl-2-
 (methylthio)ethyl]amino]carbonyl]phenyl]-1-(3-fluoro-2-pyridinyl)-3-
 (trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:566937 CAPLUS

DOCUMENT NUMBER: 142:219198

TITLE: Discovery of 1-(3'-Aminobenzisoxazol-5'-yl)-3-
 trifluoromethyl-N-[2-fluoro-4- (2'-

dimethylaminomethyl)imidazol-1-yl]phenyl]-1H-pyrazole-
 5-carboxamide Hydrochloride (Razaxaban), a Highly
 Potent, Selective, and Orally Bioavailable Factor Xa
 Inhibitor

AUTHOR(S): Quan, Mimi L.; Lam, Patrick Y. S.; Han, Qi; Pinto,
 Donald J. P.; He, Ming Y.; Li, Renhua; Ellis,
 Christopher D.; Clark, Charles G.; Teleha,

Christopher

A.; Sun, Jung-Hui; Alexander, Richard S.; Bai, Steve;
 Luetgen, Joseph M.; Knabb, Robert M.; Wong, Pancras
 C.; Wexler, Ruth R.

Corporate Source: Discovery Chemistry Pharmaceutical Research

Institute, Bristol-Myers Squibb Co., Princeton, NJ, 08543-5400,
 USA

SOURCE: Journal of Medicinal Chemistry (2005), 48(6),
 1729-1744

CODEN: JMCMAR; ISSN: 0022-2623

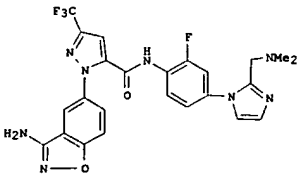
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:219198

GI



AB Modification of a series of pyrazole factor Xa inhibitors to incorporate
 an aminobenzisoxazole as the P1 ligand resulted in compds. with improved
 selectivity for factor Xa relative to trypsin and plasma kallikrein.
 Further optimization of the P4 moiety led to compds. with enhanced
 permeability and reduced protein binding. The SAR and pharmacokinetic
 profile of this series of compds. is described. These efforts culminated
 in 1-(3'-aminobenzisoxazol-5'-yl)-3-trifluoromethyl-N-[2-fluoro-4-[(2'-
 dimethylaminomethyl)imidazol-1-yl]phenyl]-1H-pyrazole-5-carboxamide (I),

a potent, selective, and orally bioavailable inhibitor of factor Xa. On
 the basis of its excellent in vitro potency and selectivity profile, high
 free fraction in human plasma, good oral bioavailability, and in vivo efficacy

10519356a.trn

L3 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

in antithrombotic models, the HCl salt of this compd. was selected for
 clin. development as razaxaban (DPC 906, BMS-561389).

IT 754193-63-0P

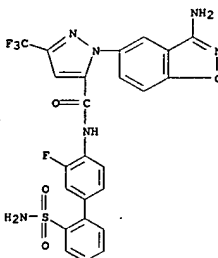
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
 (Biological study); PREP (Preparation)

(preparation of razaxaban and related compds. as potent, selective,

and orally bioavailable factor Xa inhibitors)

RN 754193-63-0 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[2'-
 (aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI)
 (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L3 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:270097 CAPLUS
 DOCUMENT NUMBER: 140:282468
 TITLE: Cloning and characterization of insect ryanodine receptors and their use for screening for insecticidal compounds
 INVENTOR(S): Caspar, Timothy; Cordova, Daniel; Gutteridge, Steven; Rauh, James J.; Smith, Rejane M.; Wu, Lihong; Tao, Yong
 PATENT ASSIGNEE(S): E. I. Du Pont de Nemours and Company, USA
 SOURCE: PCT Int. Appl., 731 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004027042	A2	20040401	WO 2003-US29834	20030923
WO 2004027042	A3	20041118		
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RM: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003275128	A1	20040408	AU 2003-275128	20030923
US 2004171114	A1	20040902	US 2003-668767	20030923
EP 1546183	A2	20050629	EP 2003-759396	20030923
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006516884	T	20060713	JP 2004-538401	20030923
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			US 2002-427324P	P 20021118
			WO 2003-US29834	W 20030923

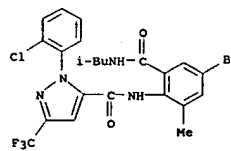
AB The genes encoding ryanodine receptor homologs are provided from multiple insect families including lepidopteran tobacco budworm (*Heliothis virescens*), homopteran green peach aphid (*Myzus persicae*), corn plant hopper (*Peregrinus maidis*), cotton melon aphid (*Aphis gossypii*), and fruitfly (*Drosophila melanogaster*). The full-length genes were isolated, cloned, and amplified in bacterial cells. Expression in insect cells shows that the recombinant protein folds into a functional calcium release channel. The genes and their corresponding polypeptides have a number of uses including, but not limited to, the isolation of other pest ryanodine receptors, the development of screens to identify insecticidally active compounds, use of fragments of genes as pesticides, fragments of protein for

L3 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:20490 CAPLUS
 DOCUMENT NUMBER: 140:77148
 TITLE: Preparation of N-[4-(thioxoheterocyclyl)phenyl]-2-phenyl-2H-pyrazole-3-carboxamides and corresponding imino-heterocyclyl derivatives as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis
 INVENTOR(S): Cezanne, Bertram; Dorsch, Dieter; Mederski, Werner; Tsakalidis, Christos; Gleitz, Johannes; Barnes, Christopher
 PATENT ASSIGNEE(S): Merck Patent GmbH, Germany
 SOURCE: PCT Int. Appl., 82 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

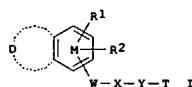
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004002477	A1	20040108	WO 2003-EP5898	20030605
WO 2004002477	A8	20040415		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RM: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10229070	A1	20040115	DE 2002-10229070	20020628
CA 2491271	A1	20040108	CA 2003-2491271	20030605
AU 2003238475	A1	20040119	AU 2003-238475	20030605
EP 1517685	A1	20050330	EP 2003-732540	20030605
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005535630	T	20051124	JP 2004-516575	20030605
EP 1679073	A1	20060712	EP 2006-157	20030605
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, SK				
US 2005203127	A1	20050915	US 2004-519356	20041228
PRIORITY APPL. INFO.:			DE 2002-10229070	A 20020628
			EP 2003-732540	A3 20030605
			WO 2003-EP5898	W 20030605

OTHER SOURCE(S): MARPAT 140:77148
 GI

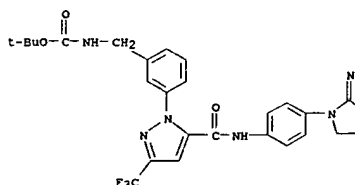
L3 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 antibody prodn., fragments of protein for detn. of the structure of insecticide binding sites, and identification of insecticides that disrupt the calcium balance in cells through other messengers that interact with the receptor calcium release mechanism. Methods are outlined for overcoming toxic effects of expressing recombinant proteins in host cells.
 IT 675826-03-6
 RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses) (cloning and characterization of insect ryanodine receptors and their use for screening for insecticidal compds.)
 RN 675826-03-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[4-bromo-2-methyl-6-[[[2-methylpropylamino]carbonyl]phenyl]-1-(2-chlorophenyl)-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)



L3 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB Title compds. [I: D = (N-, O-, S-interrupted) (substituted) C3-4 alkylene:
 M = Ph, aromatic heterocyclyl; R1, R2 = H, halo, (branched) (interrupted) (substituted) alkyl, NO2, cyano, OR3, N(R3)2, CO2R3, CON(R3)2, C(S)N(R3)2, etc.; R3 = H, (branched) (interrupted) (substituted) alkyl, etc.; W = (substituted) (bicyclic aromatic (heterocyclyl); X = CONR3, CONR3C(R4)2, C(R4)2NR3, etc.; R4 = H, (branched) (interrupted) (substituted) alkyl; Y = alkylene, cycloalkylene, heterodiy, aryldiy; T = (substituted) (bicyclic aromatic heterocyclyl), were prepared Thus, 333 mg
 (3-[5-(4-[2-iminopyrrolidin-1-yl]phenyl)carbamoyl]-3-trifluoromethylpyrazol-1-yl)benzyl)carbamoyl acid tert-Bu ester (preparation given) in EtOH was treated with HCl in ether to give 289 mg
 N-[4-(2-iminopyrrolidin-1-yl)phenyl]-1-(3-aminomethylphenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide. The latter gave affinity to the receptor Xa with IC50 = 9.6·10-9 M and to the receptor VIIa with IC50 = 2.3·10-8 M.
 IT 640288-00-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of (thioxoheterocyclyl)phenyl(pyrazole)carboxamides and corresponding imino-heterocyclyl deriva. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)
 RN 640288-00-2 CAPLUS
 CN Carbamic acid,
 [[3-[5-[[[4-(2-imino-1-pyrrolidinyl)phenyl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS

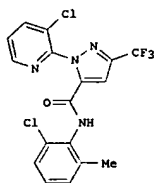
L3 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L3 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:1006958 CAPLUS
DOCUMENT NUMBER: 140:42172
TITLE: Preparation of pyrazolecarboxamide insecticides
INVENTOR(S): Stevenson, Thomas Martin; Lahm, George Philip;
Pasteris, Robert James
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003106427	A2	20031224	WO 2003-US18609	20030610
WO 2003106427	A3	20040624		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TH, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, ML, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003245464	A1	20031231	AU 2003-245464	20030610
EP 1511733	A2	20050309	EP 2003-739103	20030610
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003011707	A	20050315	BR 2003-11707	20030610
CN 1659160	A	20050824	CN 2003-812731	20030610
JP 2005532367	T	20051027	JP 2004-513260	20030610
US 2006167060	A1	20060727	US 2004-514183	20041110
PRIORITY APPL. INFO.:				US 2002-388244P P 20020613
				WO 2003-US18609 W 20030610

OTHER SOURCE(S): MARPAT 140:42172
GI

L3 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



II

AB The title compds. BNR1C((A)J [I: A = O, S; B = (un)substituted Ph, pyridinyl; J = pyrazole or pyrrole heterocyclic ring; RI = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl], useful for controlling at least one invertebrate pest (comprising contacting the invertebrate pest or its environment with a biol. effective amount of at least one compound I), were prepared E.g., a 3-step synthesis of II (starting from 2,3-dichloropyridine and 3-trifluoromethylpyrazole), was given. The compds. I were tested in 5 different tests against diamond moth, fall armyworm, tobacco budworm and beet armyworm, and biol. data were given. This invention also pertains to a composition comprising at least one compound I and at least one addnl. component selected from the group consisting of a surfactant, a solid diluent and a liquid diluent.

IT 636609-04-6P 636609-11-5P 636609-17-1P
636609-27-3P 636609-35-3P 636609-50-2P
636609-59-1P 636609-70-6P 636609-89-7P
636609-95-5P

RI: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation);

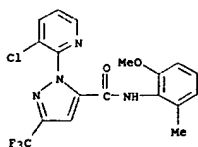
USES

(Uses)

(preparation of pyrazolecarboxamide insecticides)

RN 636609-04-6 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(2-methoxy-6-methylphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

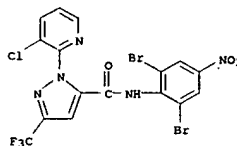


RN 636609-11-5 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(2,6-dibromo-4-

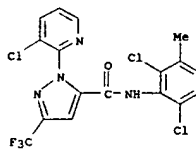
10519356a.trn

L3 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
nitrophenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



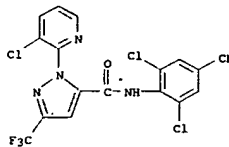
RN 636609-17-1 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(2,6-dichloro-3-methylphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 636609-27-3 CAPLUS

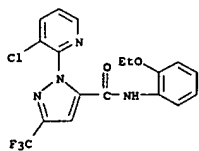
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(2,6-dichloro-4-cyanophenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



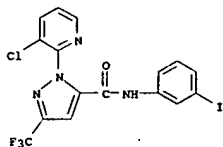
RN 636609-35-3 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(2-ethoxyphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

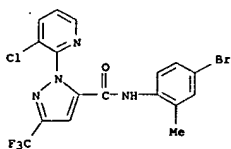
L3 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 636609-50-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(3-iodophenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 636609-59-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-(4-bromo-2-methylphenyl)-1-(3-chloro-2-pyridinyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 636609-70-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-(4-methoxyphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L3 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:844982 CAPLUS

DOCUMENT NUMBER: 140:59557

TITLE: Discovery of

1-(2-aminomethylphenyl)-3-trifluoromethyl-N-[3-fluoro-2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-1H-pyrazole-5-carboxamide (DPC602), a Potent, Selective, and Orally Bioavailable Factor Xa

Inhibitor

AUTHOR(S):
Robert

Pruitt, James R.; Pinto, Donald J. P.; Galemmo,

A., Jr.; Alexander, Richard S.; Rossi, Karen A.; Wells, Brian L.; Drummond, Spencer; Bostrom, Lori L.; Burdick, Debra; Bruckner, Robert; Chen, Haiying; Smallwood, Angela; Wong, Pancras C.; Wright, Matthew R.; Bai, Steven; Luettgen, Joseph M.; Knabb, Robert H.; Lam, Patrick Y. S.; Wexler, Ruth R.

CORPORATE SOURCE:

Pharmaceutical Research Institute, Bristol-Myers Squibb Company, Pennington, NJ, 08534, USA

SOURCE:

Journal of Medicinal Chemistry (2003), 46(25),

5298-5315

CODEN: JMCHAR; ISSN: 0022-2623

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 140:59557

AB

Factor Xa, a serine protease, is at the critical juncture between the intrinsic and extrinsic pathways of the coagulation cascade. Inhibition of factor Xa has the potential to provide effective treatment for both venous and arterial thrombosis. The authors recently described a series of meta-substituted phenylpyrazoles that are highly potent, selective,

and

orally bioavailable factor Xa inhibitors. In this paper, the authors report their efforts to further optimize the selectivity profile of the factor Xa inhibitors with a series of ortho- and/or para-substituted phenylpyrazole derivs. The most potent compds. display sub-nanomolar inhibition consts. for factor Xa and show greater than 1000-fold selectivity against other serine proteases. These compds. are also effective in a rabbit model of arteriovenous shunt thrombosis. Optimization of this series led to the preclin. development of DPC602, a 2-(aminomethyl)phenylpyrazole analog, as a highly potent, selective, and orally bioavailable factor Xa inhibitor.

IT

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of

1-(2-aminomethylphenyl)-3-trifluoromethyl-N-[3-fluoro-2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-1H-pyrazole-5-carboxamide and related compds. as orally bioavailable factor Xa inhibitors)

RN 637319-21-2 CAPLUS

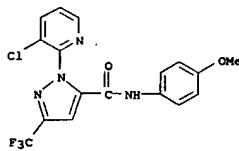
CN 1H-Pyrazole-5-carboxamide, 1-[2-(3-aminopropyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

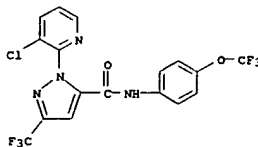
CRN 875139-45-0

CMF C27 H24 F4 N4 O3 S

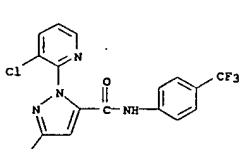
L3 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



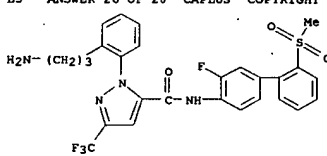
RN 636609-89-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-[4-(trifluoromethoxy)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 636609-95-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-3-(trifluoromethyl)-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1

CMF C2 H F3 O2



IT

637319-11-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

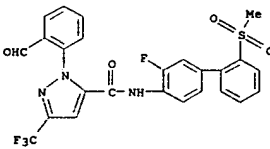
(preparation of

1-(2-aminomethylphenyl)-3-trifluoromethyl-N-[3-fluoro-2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-1H-pyrazole-5-carboxamide and related compds. as orally bioavailable factor Xa inhibitors)

RN 637319-11-0 CAPLUS

CN 1H-Pyrazole-5-carboxamide,

N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-(2-formylphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS

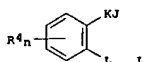
FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L3 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 ACCESSION NUMBER: 2003:261572 CAPLUS
 DOCUMENT NUMBER: 138:267208
 TITLE: Insecticidal compositions containing diamides
 INVENTOR(S): Lahm, George Philip; Selby, Thomas Paul
 PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
 SOURCE: PCT Int. Appl., 246 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003026415	A2	20030403	WO 2002-US29468	20020917
WO 2003026415	A3	20031030		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1427705	A2	20040616	EP 2002-799589	20020917
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
BR 2002012799	A	20040803	BR 2002-12799	20020917
CN 1553364	A	20041215	CN 2002-818247	20020917
JP 2005504084	T	20050210	JP 2003-530071	20020917
US 2004235959	A1	20041125	US 2004-485096	20040126
PRIORITY APPLN. INFO.:			US 2001-324083P	P 20010921
			WO 2002-US29468	W 20020917

OTHER SOURCE(S): MARPAT 138:267208
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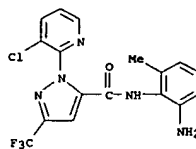
AB Comps. for controlling an invertebrate pest comprise a biol. effective amount of a compound I (Markush included), including all geometric and stereoisomers, N-oxides and agriculturally suitable salts thereof, and may optionally comprise addnl. components selected from the group consisting

L3 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 ACCESSION NUMBER: 2003:154424 CAPLUS
 DOCUMENT NUMBER: 138:205057
 TITLE: Preparation of N-[2-(heteroaryl)phenyl] pyrazole-5-carboxamides for controlling invertebrate pests
 INVENTOR(S): Clark, David Alan; Finkelstein, Bruce Lawrence; Lahm, George Philip; Selby, Tom Paul; Stevenson, Thomas Martin
 PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
 SOURCE: PCT Int. Appl., 172 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

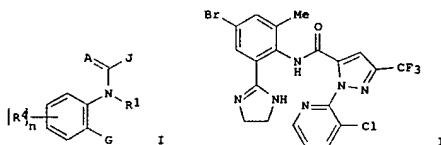
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003016304	A1	20030227	WO 2002-US26968	20020812
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RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1417204	A1	20040512	EP 2002-768688	20020812
EP 1417204	B1	20060118		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
BR 2002012186	A	20041005	BR 2002-12186	20020812
CN 1543460	A	20041103	CN 2002-815961	20020812
JP 2005502661	T	20050127	JP 2003-521227	20020812
AT 316085	T	20060215	AT 2002-768688	20020812
ES 2255624	T3	20060701	ES 2002-2768688	20020812
US 2004242645	A1	20041202	US 2004-483117	20040609
PRIORITY APPLN. INFO.:			US 2001-312440P	P 20010815
			WO 2002-US26968	W 20020812

OTHER SOURCE(S): MARPAT 138:205057
 GI

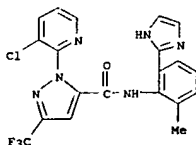
L3 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 of surfactants, solid diluents and liq. diluents, and addnl. biol. active compds. or agents selected from the group consisting of pyrethroids, carbamates, neonicotinoids, neuronal sodium channel blockers, insecticidal macrocyclic lactones, γ -aminobutyric acid (GABA) antagonists, insecticidal ureas, juvenile hormone mimics, and biol. agents. such as *Bacillus thuringiensis*, *Bt* delta endotoxins, baculoviruses, entomopathogenic bacteria, viruses and fungi.
 IT 503548-32-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of diamides as insecticide)
 RN 503548-32-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-(2-amino-6-methylphenyl)-1-(3-chloro-2-pyridinyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB The title compds. [I: A = O, S; G = (un)substituted 5-6 membered heteroarom. ring or a 5-6 membered nonarom. heterocyclic ring optionally including one or two ring members selected from the group consisting of CO, SO or SO2; J = (un)substituted Ph, a 5-6 membered heteroarom. ring or an aromatic 8-10 membered fused carbobicyclic or heterobicyclic ring system; R1 = H, alkyl, alkenyl, etc.; R4 = alkyl, alkenyl, cycloalkyl, etc.; n = 1-4], useful for controlling an invertebrate pest, were prepared. Thus, treating 1-(3-chloro-2-pyridinyl)-3-trifluoromethyl-1H-pyrazole-5-carboxylic acid with (COCl)2 in CH2Cl2 followed by addition of a solution of 4-bromo-2-(4,5-dihydro-1H-imidazol-2-yl)-6-methylbenzenamine (3-step preparation given), DMAP and Et3N in CH2Cl2 afforded II which provided excellent levels of plant protection (20% or less feeding damage) when tested at 50 ppm.
 IT 500100-88-9P
 RL: AGR (Agricultural use); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (preparation of N-[2-(heteroaryl)phenyl] pyrazole-5-carboxamides for controlling invertebrate pests)
 RN 500100-88-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-(3-chloro-2-pyridinyl)-N-[2-(1H-imidazol-2-yl)-6-methylphenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

48.37

49.03

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-7.02

-7.02

FILE 'REGISTRY' ENTERED AT 07:51:35 ON 08 JAN 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 JAN 2007 HIGHEST RN 916885-50-2

DICTIONARY FILE UPDATES: 7 JAN 2007 HIGHEST RN 916885-50-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

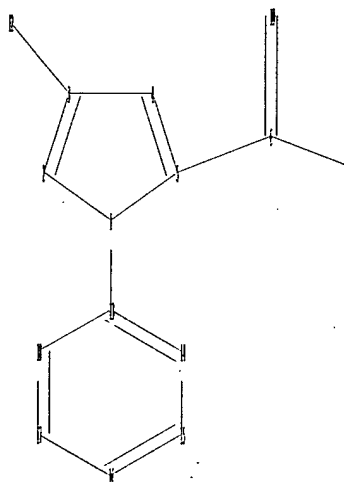
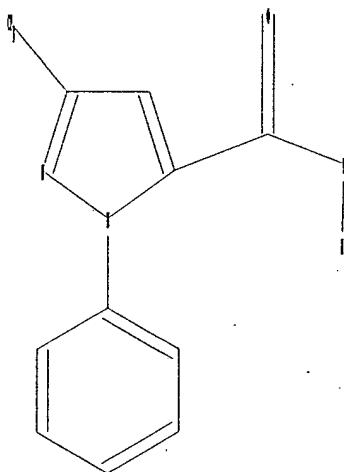
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10519356\Struc 5.str



chain nodes :

6 7 10 11 12

10519356a.trn

Page 14

ring nodes :

1 2 3 4 5 13 14 15 16 17 18

chain bonds :

1-13 3-12 5-6 6-7 6-10 7-11

ring bonds :

1-5 1-2 2-3 3-4 4-5 13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds :

1-5 1-2 1-13 2-3 3-4 4-5 6-7 6-10

exact bonds :

3-12 5-6 7-11

normalized bonds :

13-14 13-18 14-15 15-16 16-17 17-18

G1:Cb,Cy,Hy

G2:S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 10:CLASS 11:CLASS

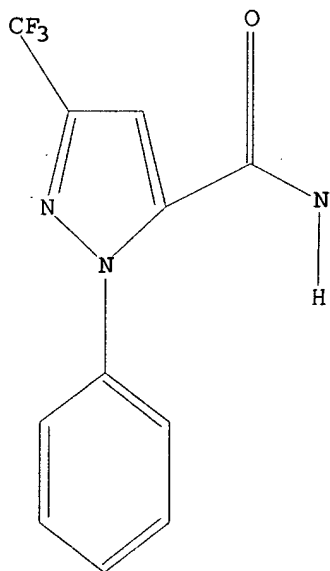
12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom

L4 STRUCTURE UPLOADED

=> d

L4 HAS NO ANSWERS

L4 STR



G1 Cb,Cy,Hy

G2 S,N

10519356a.trn

Structure attributes must be viewed using STN Express query preparation.

=> 14

SAMPLE SEARCH INITIATED 07:52:31 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 132 TO ITERATE

100.0% PROCESSED 132 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1951 TO 3329

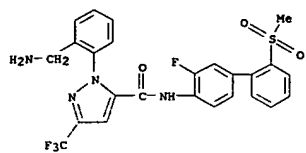
PROJECTED ANSWERS: 752 TO 1688

L5 50 SEA SSS SAM L4

=> d scan

L5 50 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 1H-Pyrazole-5-carboxamide, 1-(2-(aminomethyl)phenyl)-N-(3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl)-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI)
 MF C25 H20 F4 N4 O3 S . C2 H F3 O2

CH 1



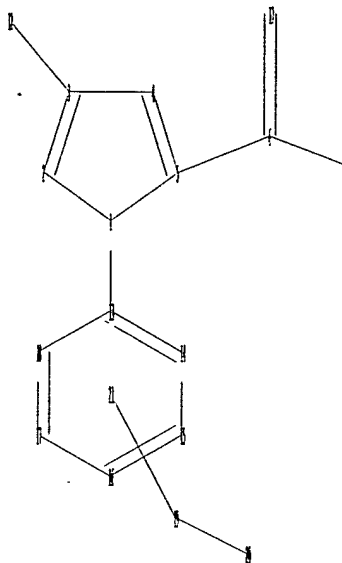
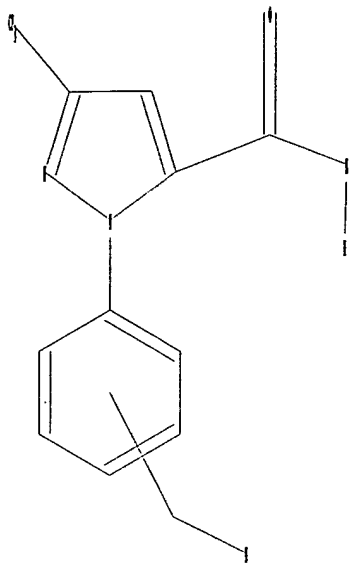
CH 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>

Uploading C:\Program Files\Stnexp\Queries\10519356\Struc 6.str



chain nodes :

6 7 10 11 12 19 20

ring nodes :

1 2 3 4 5 13 14 15 16 17 18

chain bonds :

1-13 3-12 5-6 6-7 6-10 7-11 19-20

ring bonds :

1-5 1-2 2-3 3-4 4-5 13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds :

1-5 1-2 1-13 2-3 3-4 4-5 6-7 6-10 19-20

exact bonds :

3-12 5-6 7-11

normalized bonds :

13-14 13-18 14-15 15-16 16-17 17-18

G1:Cb,Cy,Hy

G2:S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 10:CLASS 11:CLASS

12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS :

21:Atom

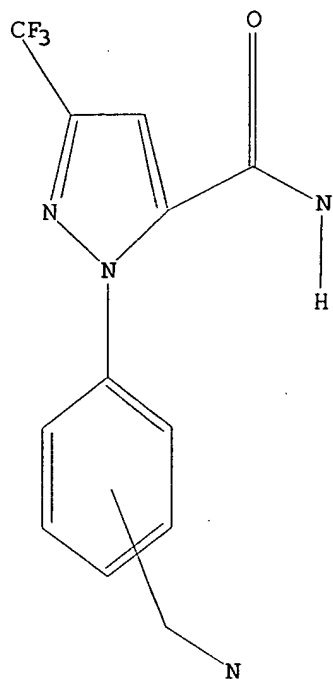
L6 STRUCTURE UPLOADED

=> d

L6 HAS NO ANSWERS

L6 STR

10519356a.trn



G1 Cb,Cy,Hy

G2 S,N

Structure attributes must be viewed using STN Express query preparation.

=> 16

SAMPLE SEARCH INITIATED 07:55:59 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 132 TO ITERATE

100.0% PROCESSED 132 ITERATIONS

22 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 1951 TO 3329

PROJECTED ANSWERS: 159 TO 721

L7 22 SEA SSS SAM L6

=> 16 full

FULL SEARCH INITIATED 07:56:04 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 2606 TO ITERATE

100.0% PROCESSED 2606 ITERATIONS

426 ANSWERS

SEARCH TIME: 00.00.01

L8 426 SEA SSS FUL L6

10519356a.trn

Page 19

=> file medline caplus
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
175.25	224.28

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-7.02

CA SUBSCRIBER PRICE

FILE 'MEDLINE' ENTERED AT 07:56:10 ON 08 JAN 2007

FILE 'CAPLUS' ENTERED AT 07:56:10 ON 08 JAN 2007

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=> 18

L9 36 L8

=> d ibib abs hitstr 1-36

L9 ANSWER 1 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1096816 CAPLUS
 DOCUMENT NUMBER: 145:443880
 TITLE: Odiparcil and a factor Xa inhibitor formulations for treatment of thromboembolic disorders
 INVENTOR(S): Ohlstein, Eliot H.
 PATENT ASSIGNEE(S): Glaxo Group Limited, UK
 SOURCE: PCT Int. Appl., 42pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006110726	A2	20061019	WO 2006-US13448	20060411
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.: US 2005-66985P P 20050411

OTHER SOURCE(S): MARPAT 145:443880
 AB The present invention relates to combinations of 4-methyl-2-oxo-2H-1-benzopyran-7-yl-5-thio-β-D-xylopyranoside (odiparcil) and factor Xa inhibitors, methods for producing the combinations, and methods of using the combinations for the treatment and prevention of various thromboembolic disorders in mammals, particularly humans. Thus, 2 parts odiparcil are combined with 1 part by weight rivaroxaban. The combined powders are then optionally milled to desired particle size range. The combination of the 2 drugs is then further combined with a wetting agent, disintegrant and/or filler and compressed into tablets of the following strengths: 50 mg odiparcil/25 mg rivaroxaban; 100 mg odiparcil/50 mg rivaroxaban; 200 mg odiparcil/100 mg rivaroxaban; 250 mg odiparcil/125 mg rivaroxaban.
 IT 228258-45-5, DPC 602 292135-59-2, DPC 423
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (odiparcil and factor Xa inhibitor formulations for treatment of thromboembolic disorders)
 RN 228258-45-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

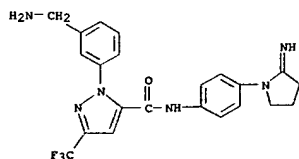
L9 ANSWER 2 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1061760 CAPLUS
 TITLE: Design and Evaluation of a Novel Class-Directed 2D Fingerprint to Search for Structurally Diverse Active Compounds
 AUTHOR(S): Eckert, Hanna; Bajorath, Juergen
 CORPORATE SOURCE: Department of Life Science Informatics, B-IT, Rheinische Friedrich-Wilhelms-Universitaet, Bonn, D-53113, Germany
 SOURCE: Journal of Chemical Information and Modeling (2006), 46(6), 2515-2526
 CODEN: JCISD8; ISSN: 1549-9596
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

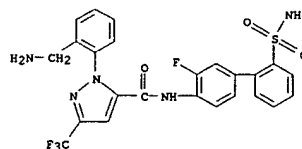
AB Recent attempts to increase similarity search performance using mol. fingerprints have mostly focused on the evaluation of alternative similarity metrics or scoring schemes, rather than the development of new types of fingerprints. Here, the authors introduce a novel 2D fingerprint design (property descriptor value range-derived fingerprint or PDR-FP) that involves activity-oriented selection of property descriptors and the transformation of descriptor value ranges into a binary format such that each fingerprint bit position represents a specific value interval. The design is tailored toward multiple-template similarity searching and permits training on specific activity classes. In search calcs. on 15 compound classes of increasing structural diversity, the PDR fingerprint performed better than other state-of-the-art 2D fingerprints. Among the structurally diverse classes were six compound sets with peptide character, which represent a notoriously difficult chemotype for 2D similarity searching. In these cases, PDR-FP produced promising results, whereas other fingerprint methods mostly failed. PDR-FP is specifically designed for search calcs. on structurally diverse compds., and these calcs. are not influenced by mol. size effects, which represent a general problem

for similarity searching using bit string representations.
 IT 774536-86-6
 RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PRP (Properties); USES (Uses) (design and evaluation of a class-directed 2D fingerprint to search

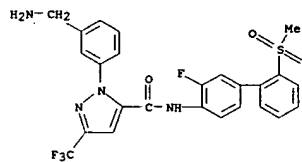
for structurally diverse active compds.)
 RN 774536-86-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 1 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 292135-59-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L9 ANSWER 2 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 ACCESSION NUMBER: 2006:635022 CAPLUS
 DOCUMENT NUMBER: 145:103950
 TITLE: Preparation of amino acid derivatives as inhibitors of
 protein arginine methyl transferases
 INVENTOR(S): Purandare, Ashok Vinayak; Chen, Zhong
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
 SOURCE: PCT Int. Appl., 125 pp.
 CODEN: PIXOXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

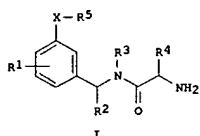
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006069155	A2	20060629	WO 2005-US46362	20051221
WO 2006069155	A3	20061123		

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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

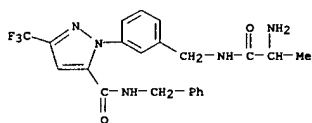
PRIORITY APPLN. INFO.: US 2004-637893P P 20041221

OTHER SOURCE(S): MARPAT 145:103950
 GI



AB The invention relates to compds. I [X is Ph or 5-membered heteroaryl; R1 is H, halogen, CN, alkyl or substituted alkyl, alkoxy, alkylthio, or alkylsulfonyl; R2 is H or alkyl; R3 is H, Me, or Et; R4 is H, Me, Et, iso-Pr, CH2Ph, OH, or OPh; or R3 and R4 may form a 5- or 6-membered

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
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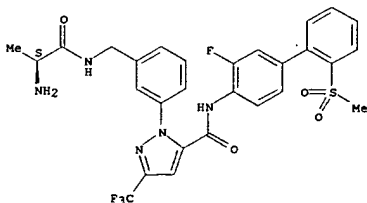


CM 2
 CRN 76-05-1
 CMF C2 H F3 O2



RN 895522-43-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 895522-44-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2R)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 heterocycle; R5 is -W-(CH2)0-3-O0-1-R6, where W is CONH, 1,3,4-oxadiazole-2,5-diyl, etc and R6 is (un)substituted cycloalkyl, heterocyclyl, or aryl or a stereoisomer, tautomer, or pharmaceutically-acceptable salt and their use in the treatment of hyperproliferative, inflammatory, infectious, and immunoregulatory disorders and diseases. Thus, 1 [R1-R3 = H, R4 = Me, R5-X = 5-(benzylcarbamoyl)-3-(trifluoromethyl)-1-pyrazolyl] was prepd. from 1-(3-cyanophenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxylic acid by hydrogenation over Pd/C, followed by amidation reactions with Boc-Ala-OSu and benzylamine. The product was assayed for inhibition of tumor cell proliferation using the 3H thymidine incorporation protocol (IC50 < 10 μM)

IT 895522-42-6P 895522-43-7P 895522-44-8P
 895522-45-9P 895522-46-0P 895522-47-1P
 895522-49-3P 895522-51-7P 895522-56-2P
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 895523-26-9P 895523-27-0P 895523-28-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amino acid derivs. as inhibitors of protein arginine

Me transferases)

RN 895522-42-6 CAPLUS

CN 1H-Pyrazole-5-carboxamide,

1-[3-[[[(2-amino-1-oxopropyl)amino]methyl]phenyl

]N-(phenylmethyl)-3-(trifluoroacetate) (9CI)

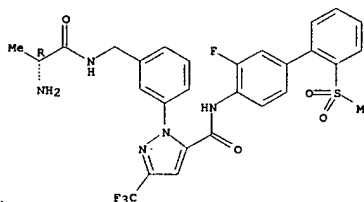
(CA

INDEX NAME)

CH 1

CRN 895522-41-5

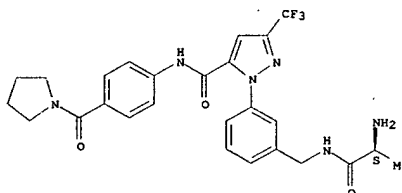
L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-45-9 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

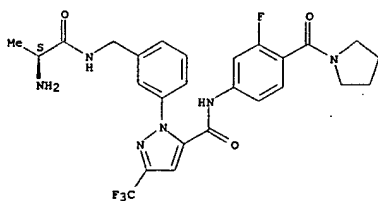


RN 895522-46-0 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[3-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

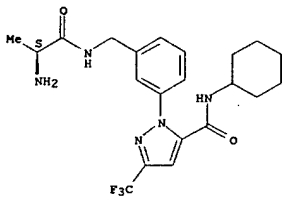
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-47-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-cyclohexyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



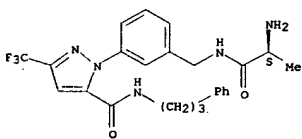
RN 895522-49-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-phenyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

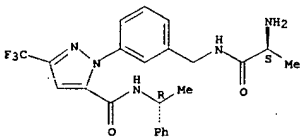
RN 895522-57-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(3-phenylpropyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



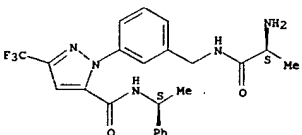
RN 895522-58-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(1R)-1-phenylethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

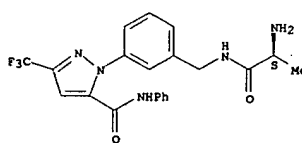


RN 895522-59-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(1S)-1-phenylethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

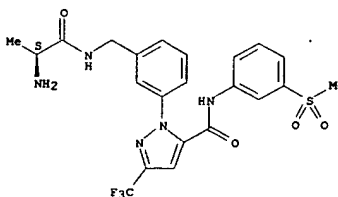


L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



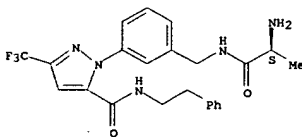
RN 895522-51-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2S)-2-amino-1-oxopropyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 895522-56-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(2-phenylethyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

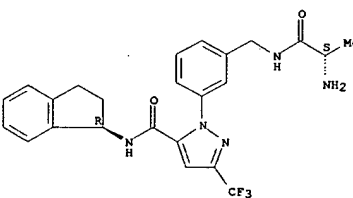
Absolute stereochemistry.



L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

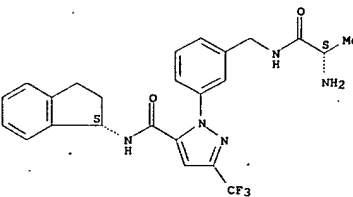
RN 895522-60-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(1R)-2,3-dihydro-1H-inden-1-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 895522-61-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(1S)-2,3-dihydro-1H-inden-1-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

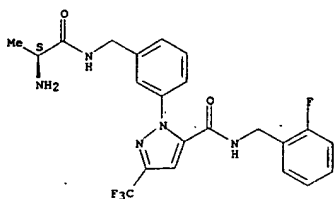
Absolute stereochemistry.



RN 895522-62-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2S)-2-amino-1-oxopropyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

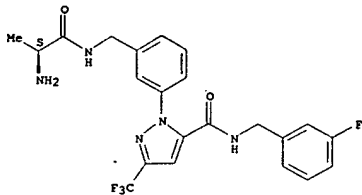
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-63-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(3-fluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

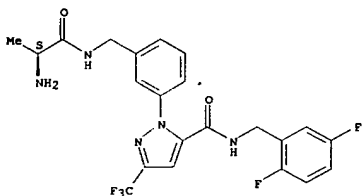
Absolute stereochemistry.



RN 895522-64-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(4-fluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

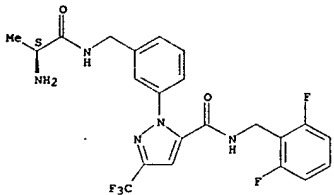
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-67-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2,6-difluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

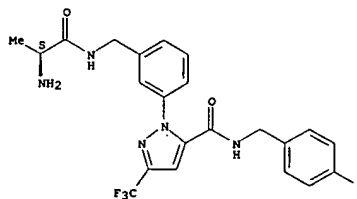
Absolute stereochemistry.



RN 895522-68-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(3,4-difluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

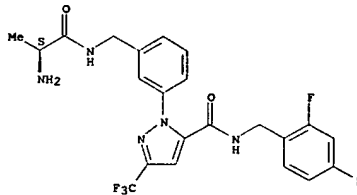
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-65-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2,4-difluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

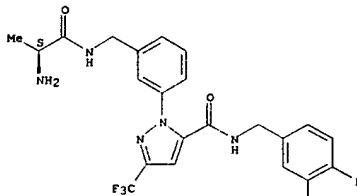
Absolute stereochemistry.



RN 895522-66-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2,5-difluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

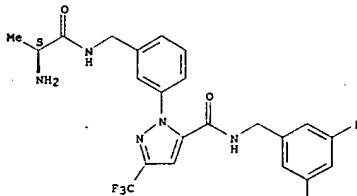
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-69-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(3,5-difluorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

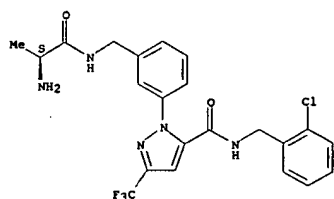
Absolute stereochemistry.



RN 895522-70-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2-chlorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

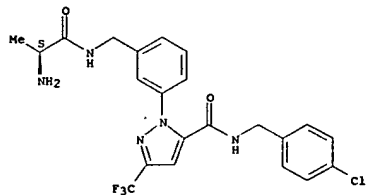
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-71-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(4-chlorophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

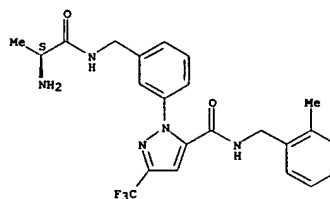
Absolute stereochemistry.



RN 895522-72-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2-methylphenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

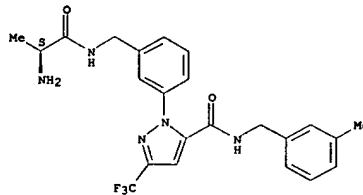
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-73-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(3-methylphenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

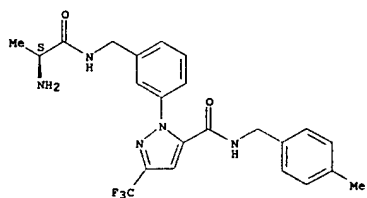
Absolute stereochemistry.



RN 895522-74-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(4-methylphenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

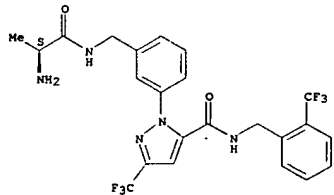
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-75-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-N-[(2-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

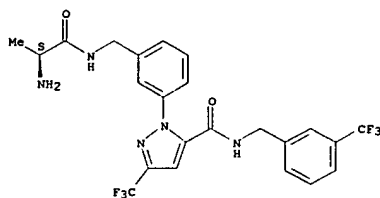
Absolute stereochemistry.



RN 895522-76-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-N-[(2-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

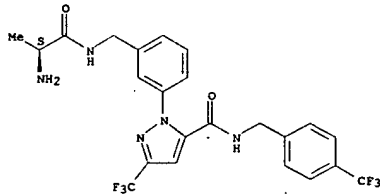
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-77-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-N-[(4-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

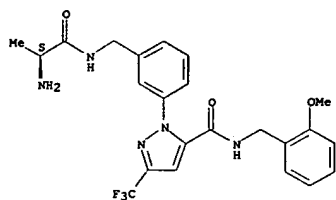
Absolute stereochemistry.



RN 895522-78-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2-methoxyphenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

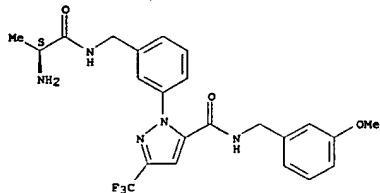
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-79-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(3-methoxyphenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

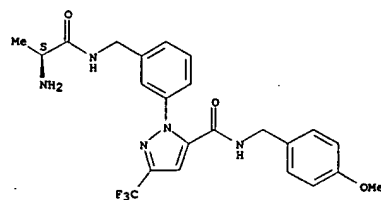
Absolute stereochemistry.



RN 895522-80-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(4-methoxyphenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

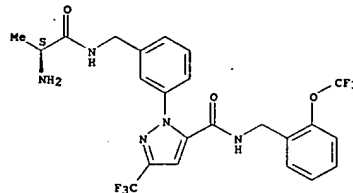
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-81-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[[2-(trifluoromethoxy)phenyl]methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

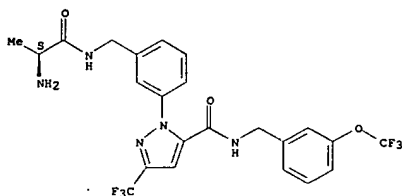
Absolute stereochemistry.



RN 895522-82-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[[3-(trifluoromethoxy)phenyl]methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

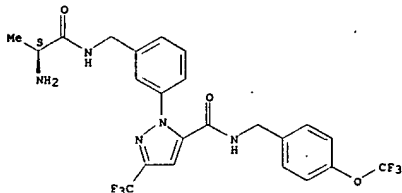
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-83-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[[4-(trifluoromethoxy)phenyl]methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

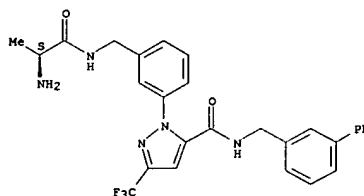
Absolute stereochemistry.



RN 895522-84-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[[1,1'-biphenyl]-3-ylmethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

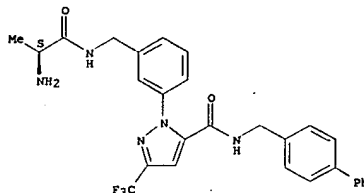
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-85-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[[1,1'-biphenyl]-4-ylmethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

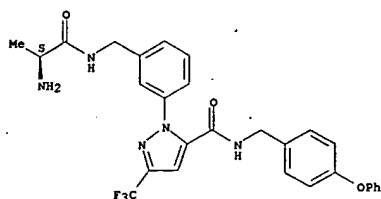
Absolute stereochemistry.



RN 895522-86-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[[4-(phenoxymethyl)phenyl]methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

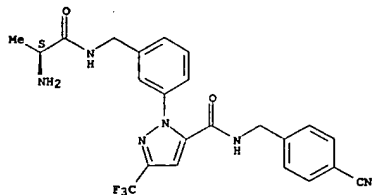
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-87-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(4-cyanophenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

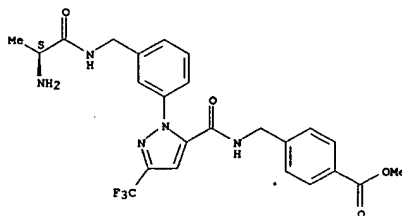
Absolute stereochemistry.



RN 895522-88-0 CAPLUS
 CN Benzoic acid, 4-[[[1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

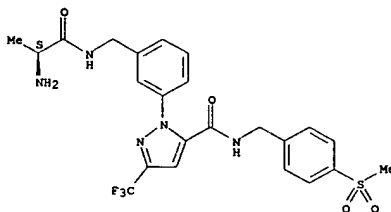
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-89-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(4-methylsulfonyl)phenyl]methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

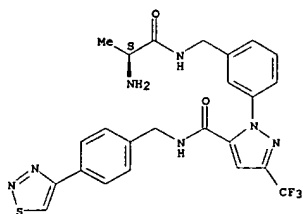
Absolute stereochemistry.



RN 895522-90-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(1,2,3-thiadiazol-4-yl)phenyl]methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

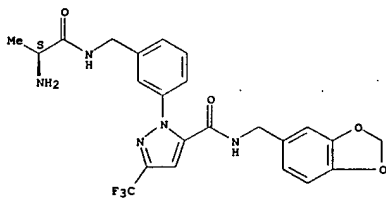
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-91-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(1,3-benzodioxol-5-yl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

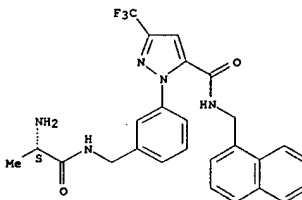
Absolute stereochemistry.



RN 895522-92-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(1-naphthalenyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

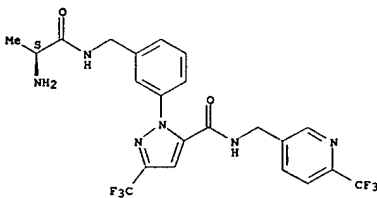
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-93-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-N-[(6-(trifluoromethyl)-3-pyridinyl)methyl]- (9CI) (CA INDEX NAME)

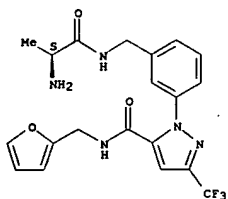
Absolute stereochemistry.



RN 895522-94-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(2-furanylmethyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

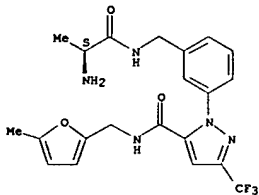
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-95-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(5-methyl-2-furanyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

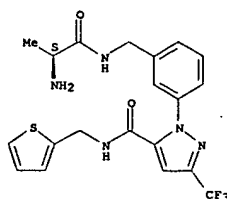
Absolute stereochemistry.



RN 895522-96-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2-thienyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

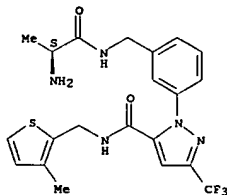
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-97-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(3-methyl-2-thienyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

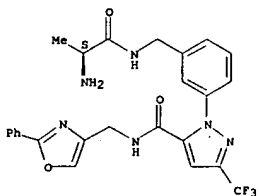
Absolute stereochemistry.



RN 895522-98-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2-phenyl-4-oxazolyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

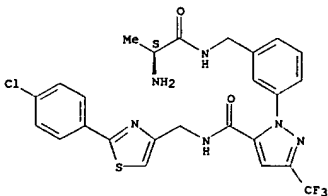
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895522-99-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(2-(4-chlorophenyl)-4-thiazolyl)methyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

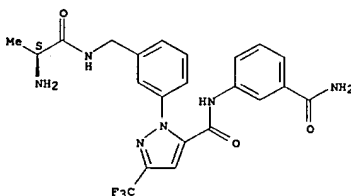
Absolute stereochemistry.



RN 895523-00-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[(3-(aminocarbonyl)phenyl)-1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

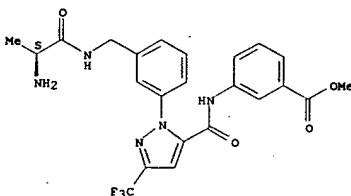
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-01-0 CAPLUS
 CN Benzoic acid, 3-[[[1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

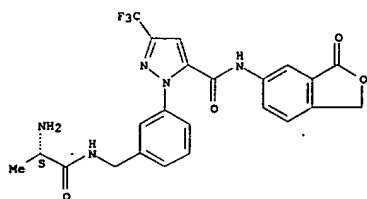
Absolute stereochemistry.



RN 895523-02-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[(1,3-dihydro-3-oxo-5-isobenzofuranyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

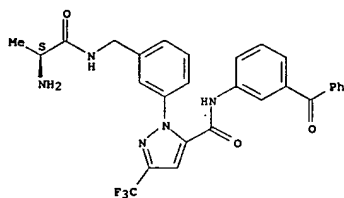
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-03-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(3-benzoylphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

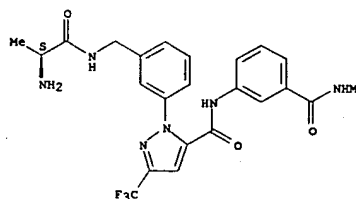
Absolute stereochemistry.



RN 895523-04-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(3-[(methylamino)carbonyl]phenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

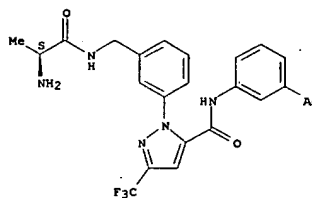
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-05-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-(3-acetylphenyl)-1-[3-[[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

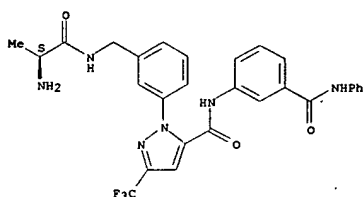
Absolute stereochemistry.



RN 895523-06-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(3-[(phenylamino)carbonyl]phenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

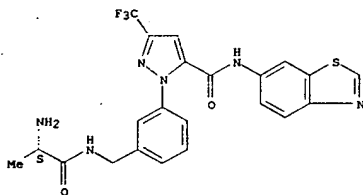
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-07-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(2-methyl-5-benzothiazolyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

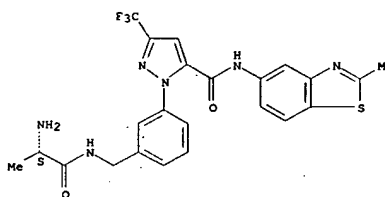
Absolute stereochemistry.



RN 895523-08-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(2-methyl-5-benzothiazolyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

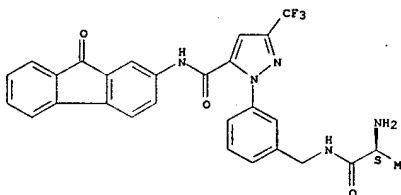
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-09-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(9-oxo-9H-fluoren-2-yl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

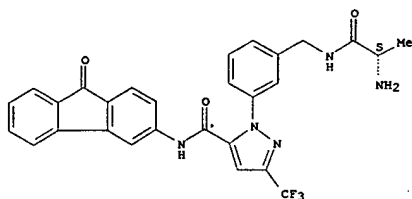
Absolute stereochemistry.



RN 895523-10-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(9-oxo-9H-fluoren-3-yl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

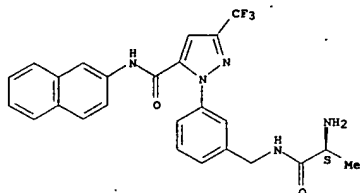
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-11-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-2-naphthalenyl-3-(trifluoromethyl)- (9CI)
 (CA INDEX NAME)

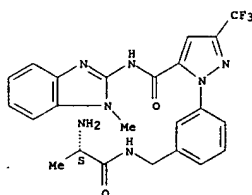
Absolute stereochemistry.



RN 895523-12-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-6-quinolinyl-3-(trifluoromethyl)- (9CI)
 (CA INDEX NAME)

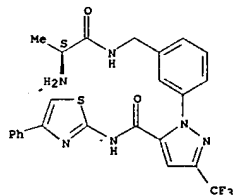
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-15-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(4-phenyl-2-thiazolyl)-3-(trifluoromethyl)- (9CI)
 (CA INDEX NAME)

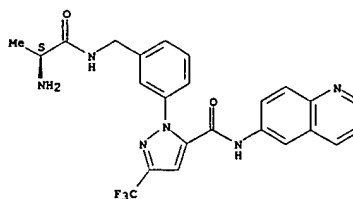
Absolute stereochemistry.



RN 895523-16-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-2-thiazolyl-3-(trifluoromethyl)- (9CI)
 (CA INDEX NAME)

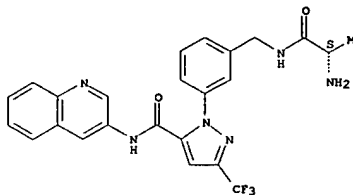
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-13-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-3-quinolinyl-3-(trifluoromethyl)- (9CI)
 (CA INDEX NAME)

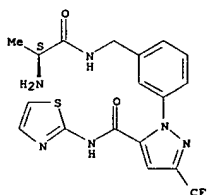
Absolute stereochemistry.



RN 895523-14-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(1-methyl-1H-benzimidazol-2-yl)-3-(trifluoromethyl)- (9CI)
 (CA INDEX NAME)

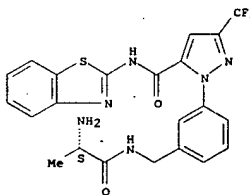
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-17-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-2-benzothiazolyl-3-(trifluoromethyl)- (9CI)
 (CA INDEX NAME)

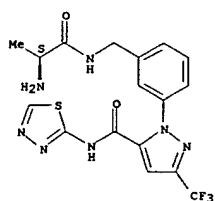
Absolute stereochemistry.



RN 895523-18-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-1,3,4-thiadiazol-2-yl-3-(trifluoromethyl)- (9CI)
 (CA INDEX NAME)

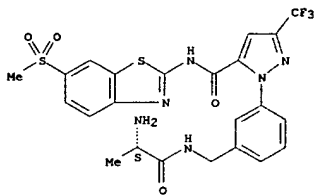
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-19-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-[6-(methylsulfonyl)-2-benzothiazolyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

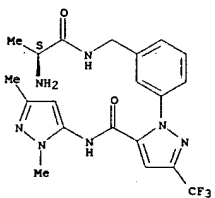
Absolute stereochemistry.



RN 895523-20-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-(5-acetyl-4-methyl-2-thiazolyl)-1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

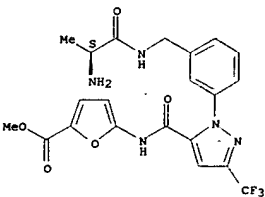
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-23-6 CAPLUS
 CN 2-Furancarboxylic acid, 5-[[[1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

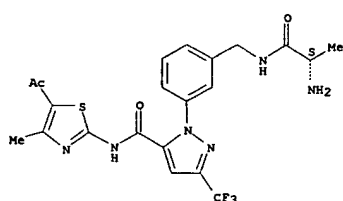
Absolute stereochemistry.



RN 895523-24-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(1-methyl-3-phenyl-1H-pyrazol-5-yl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

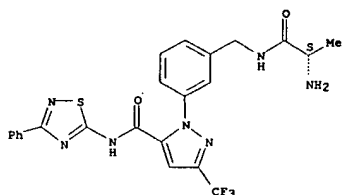
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-21-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(1,3-dimethyl-1H-pyrazol-5-yl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

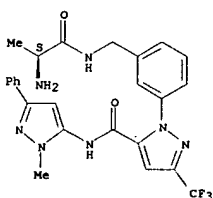
Absolute stereochemistry.



RN 895523-22-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(1,3-dimethyl-1H-pyrazol-5-yl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

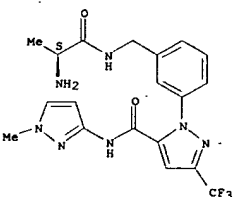
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895523-25-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(1-methyl-3-phenyl-1H-pyrazol-5-yl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

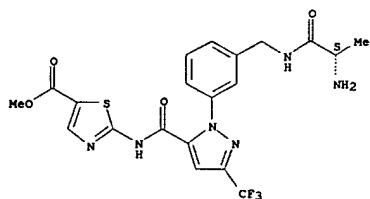
Absolute stereochemistry.



RN 895523-26-9 CAPLUS
 CN 5-Thiazolecarboxylic acid, 2-[[[1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

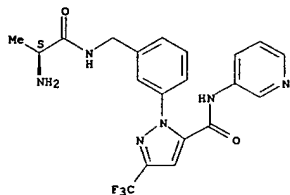
Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)



RN 895523-27-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(3-pyridinyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

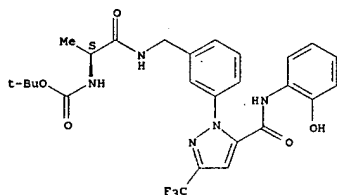
Absolute stereochemistry.



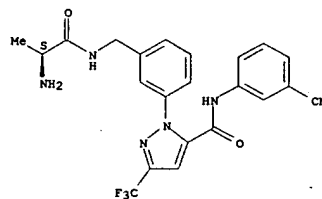
RN 895523-28-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-[[[(2S)-2-amino-1-oxopropyl]amino]methyl]phenyl]-N-(3-cyanophenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)



L9 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)

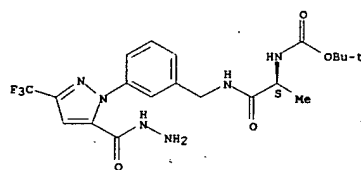


IT 895524-51-3P 895524-53-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of amino acid derivs. as inhibitors of protein arginine

Me transferases)
 RN 895524-51-3 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 1-[3-[[[(2S)-2-[[[1,1-dimethylethoxy]carbonyl]amino]-1-oxopropyl]amino]methyl]phenyl]-3-(trifluoromethyl)-, hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 895524-53-5 CAPLUS
 CN Carbanic acid, [(1S)-2-[[[3-[5-[[[(2-hydroxyphenyl)amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]amino]-1-methyl-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

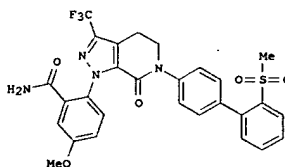
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 2006:388784 CAPLUS
 DOCUMENT NUMBER: 144:432799
 TITLE: Preparation of pyrazolylbenzamides and pyrazolopyridinylbenzamides as factor Xa inhibitors for the treatment of thromboembolic disorders
 INVENTOR(S): Lam, Patrick Y.; Clark, Charles G.; Li, Renhua;
 Haque,
 PATENT ASSIGNEE(S): Tasir S.; Rossi, Karen A.
 SOURCE: U.S. Pat. Appl. Publ., 178 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006089496	A1	20060427	US 2005-256893	20051024
WO 2006047528	A2	20060504	WO 2005-US38401	20051025
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
PRIORITY APPLN. INFO.:			US 2004-622236P	P 20041026
			US 2005-256893	A 20051024

OTHER SOURCE(S): MARPAT 144:432799

GI



II

AB Title compds. and analogs I P4-P-M-M4 (wherein M = certain carbocycle or heterocycle; P (fused onto ring M) = certain carbocycle or heterocycle;

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
when P is absent P4 and M4 are directly attached to the 1,2, 1,3 and 1,4 positions of ring M; P4 = 2-(aminocarbonyl)phenyl, etc.; M4 = methylsulfonylbiphenyl, etc.; esp. pyrazolylbenzamides and pyrazolopyridinylbenzamides such as 11, and stereoisomers, pharmaceutically acceptable salts or solvate forms thereof were prepd. as factor Xa inhibitors. A no. of the invented compds. were found to exhibit

Ki of ≤ 10 μ M against purified human factor Xa. Therefore, 1 and their pharmaceutical compns. are useful for the treatment of thromboembolic disorders.

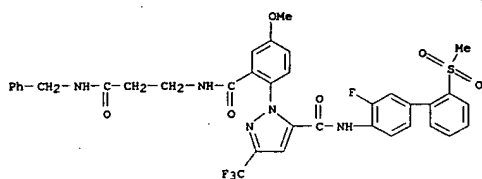
IT 885022-19-5P 885022-21-9P 885022-23-1P
885022-25-3P 885022-27-5P 885022-29-7P
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885022-37-7P 885022-39-9P 885022-41-3P
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885022-52-6P 885022-54-8P 885022-55-9P
885022-57-1P 885022-58-2P 885022-59-3P
885022-60-6P 885022-61-7P 885022-63-9P
885022-65-1P 885022-67-3P 885022-69-5P
885022-70-8P 885022-71-9P 885022-73-1P
885022-74-2P 885022-75-3P 885022-76-4P
885022-77-5P 885022-79-7P 885022-80-0P
885022-81-1P 885022-82-2P 885022-83-3P
885022-84-4P 885022-87-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of pyrazolylbenzamides and pyrazolopyridinylbenzamides as factor Xa inhibitors for treatment of thromboembolic disorders)

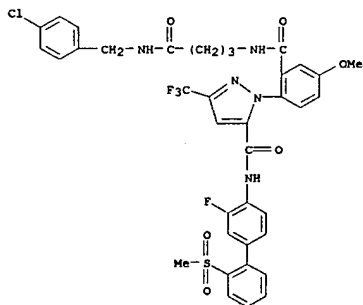
RN 885022-19-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)(1,1'-biphenyl)-

4-yl]-1-[4-methoxy-2-[[[3-oxo-3-[(phenylmethyl)amino]propyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 885022-21-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)(1,1'-biphenyl)-

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

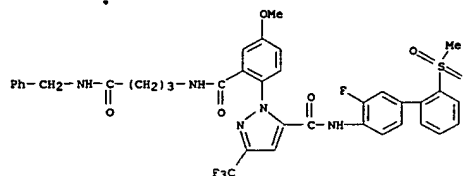


RN 885022-27-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-[[[1S]-2-[[[4-chlorophenyl)methyl]amino]-1-methyl-2-oxoethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)(1,1'-biphenyl)-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

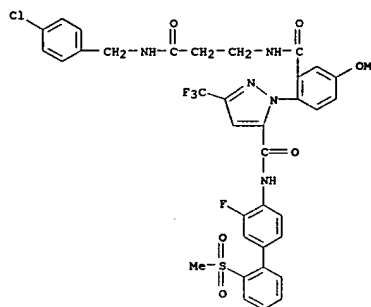
Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

4-yl]-1-[4-methoxy-2-[[[4-oxo-4-[(phenylmethyl)amino]butyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

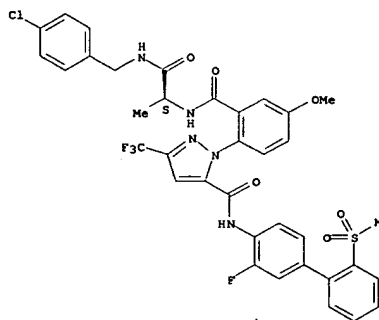


RN 885022-23-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[1S]-2-[[[4-chlorophenyl)methyl]amino]-3-oxopropyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)(1,1'-biphenyl)-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 885022-25-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[1S]-2-[[[4-chlorophenyl)methyl]amino]-4-oxobutyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)(1,1'-biphenyl)-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

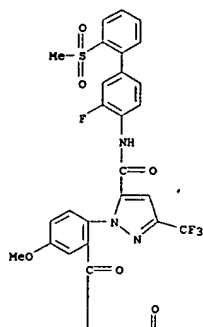
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



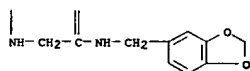
RN 885022-29-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-[[[1S]-2-[[[1,3-benzodioxol-5-ylmethyl]amino]-2-oxoethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)(1,1'-biphenyl)-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

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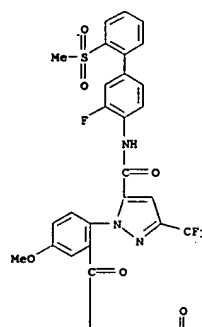
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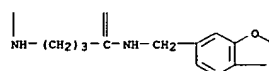
RN 885022-31-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[4-[(1,3-benzodioxol-5-ylmethyl)amino]-4-oxobutyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

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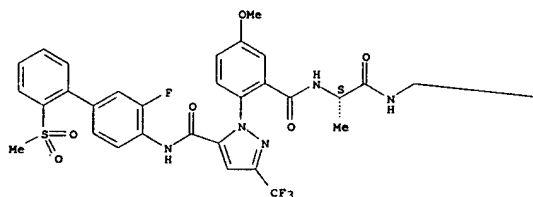


RN 885022-33-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[1S]-2-[(1,3-benzodioxol-5-ylmethyl)amino]-1-methyl-2-oxoethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

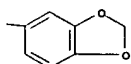
Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

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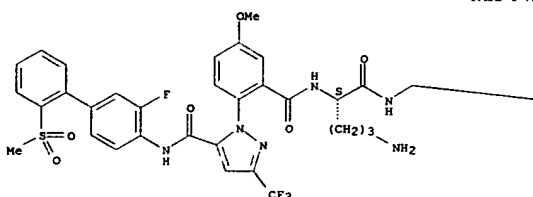
PAGE 1-B



RN 885022-35-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[1S]-4-amino-1-[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]butyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

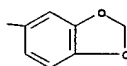
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L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

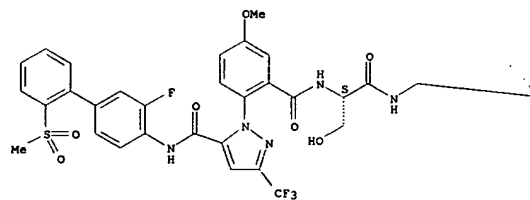
PAGE 1-B



RN 885022-37-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[1S]-2-[(1,3-benzodioxol-5-ylmethyl)amino]-1-(hydroxymethyl)-2-oxoethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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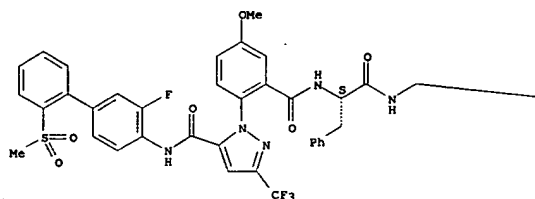


RN 885022-39-9 CAPLUS

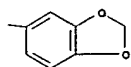
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[1,3-benzodioxol-5-ylmethyl]amino]-2-oxo-1-(phenylmethyl)ethyl]amino]carbonyl-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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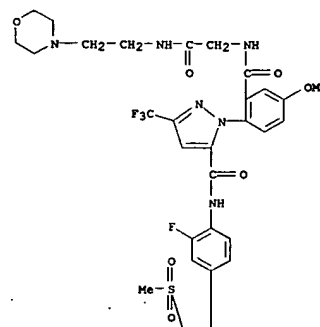
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RN 885022-41-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[[[2-[(4-morpholinyl)ethyl]amino]-3-oxoethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

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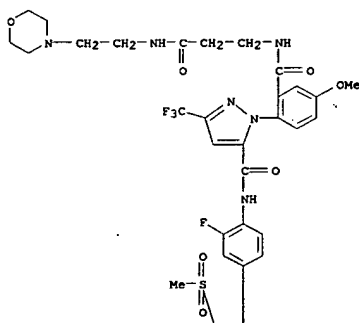
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RN 885022-43-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[[[3-[[2-(4-morpholinyl)ethyl]amino]-3-oxopropyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

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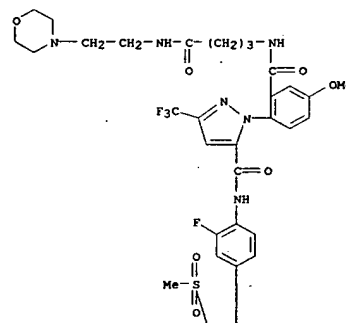
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RN 885022-45-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[[[4-[[2-(4-morpholinyl)ethyl]amino]-4-oxobutyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

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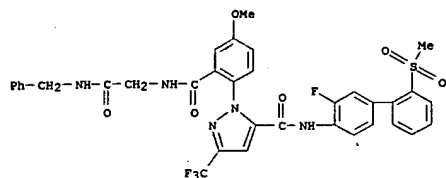


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RN 885022-47-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-[[[2-oxo-2-[(phenylmethyl)amino]ethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



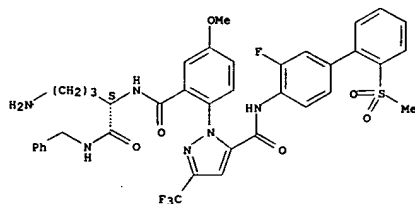
RN 885022-49-1 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[2-(((1S)-4-amino-1-

((phenylmethyl)amino)carbonyl)butyl)amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI)

(CA INDEX NAME)

Absolute stereochemistry.



RN 885022-50-4 CAPLUS

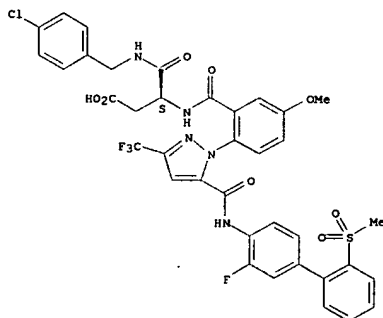
CN 1H-Pyrazole-5-carboxamide,

N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-(((1S)-2-oxo-1-(phenylmethyl)-2-((phenylmethyl)amino)ethyl)amino)carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry.



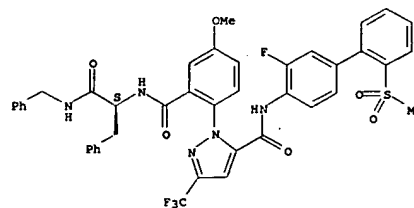
RN 885022-54-8 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[2-(((1S)-4-amino-1-(((4-

chlorophenyl)methyl)amino)carbonyl)butyl)amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

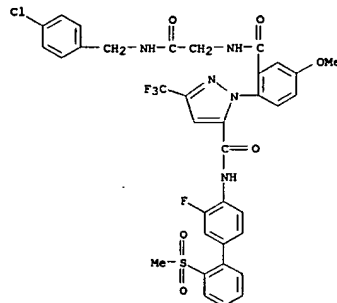
Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-51-5 CAPLUS

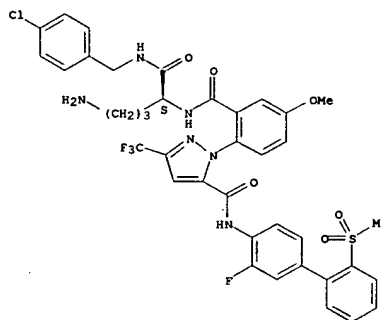
CN 1H-Pyrazole-5-carboxamide, 1-[2-(((1S)-4-amino-1-(((4-chlorophenyl)methyl)amino)carbonyl)butyl)amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 885022-52-6 CAPLUS

CN Butanoic acid, 4-(((4-chlorophenyl)methyl)amino)-3-([2-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]-5-methoxybenzoyl)amino)-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-55-9 CAPLUS

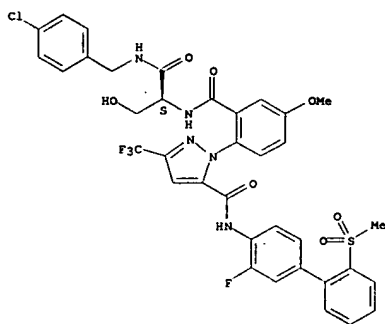
CN 1H-Pyrazole-5-carboxamide,

1-[2-(((1S)-2-(((4-chlorophenyl)methyl)amino)-

1-(hydroxymethyl)-2-oxoethyl)amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

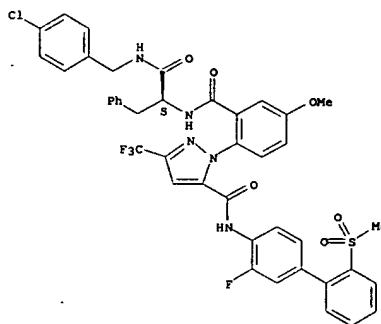
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-57-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 1-[2-[[[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-2'-oxo-1-(phenylmethyl)ethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)]-1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

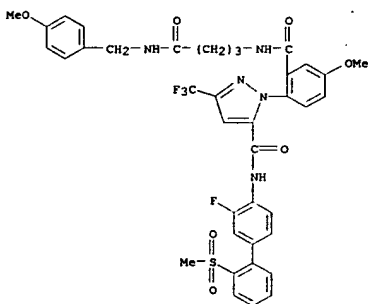
Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

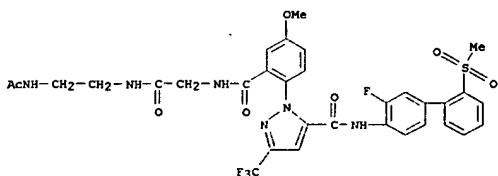


RN 885022-58-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)]-1,1'-biphenyl]-4-yl]-1-[4-methoxy-2'-[[[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-2'-oxo-1-(phenylmethyl)ethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

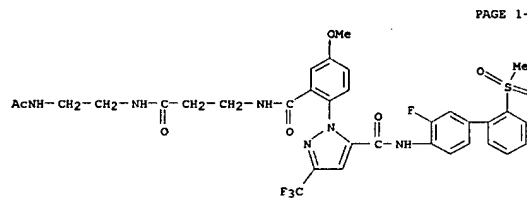


RN 885022-59-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[2-(acetylamino)ethyl]amino]-2-oxoethyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)]-1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 885022-60-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[3-[[2-(acetylamino)ethyl]amino]-3-oxopropyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)]-1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

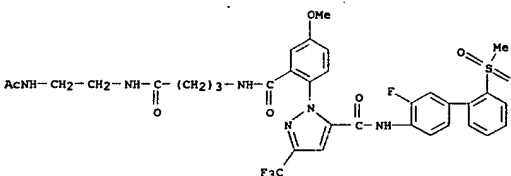


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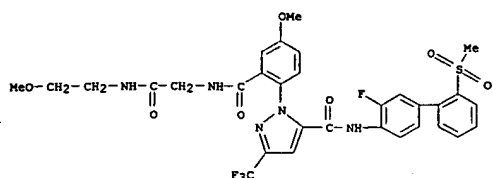
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RN 885022-61-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[4-[[2-(acetylamino)ethyl]amino]-4-oxobutyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)]-1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

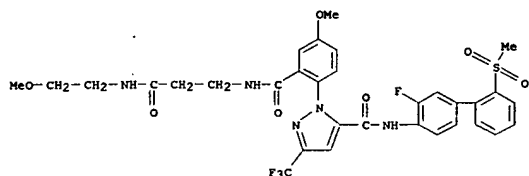


RN 885022-63-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)]-1,1'-biphenyl]-4-yl]-1-[4-methoxy-2'-[[[2-[[2-(acetylamino)ethyl]amino]-2-oxoethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

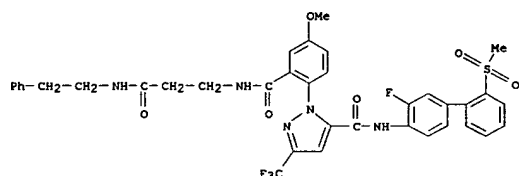


RN 885022-65-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
 4-yl]-1-[4-methoxy-2-[[[3-[(2-methoxyethyl)amino]-3-oxopropyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

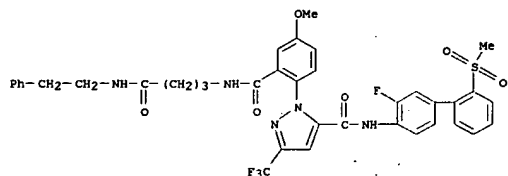


RN 885022-67-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
 4-yl]-1-[4-methoxy-2-[[[4-[(2-methoxyethyl)amino]-4-oxobutyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



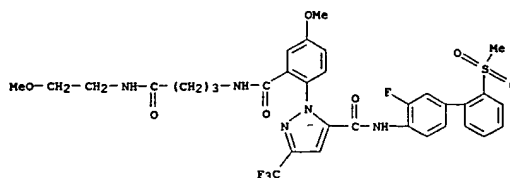
RN 885022-71-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
 4-yl]-1-[4-methoxy-2-[[[4-oxo-4-[(2-phenylethyl)amino]butyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



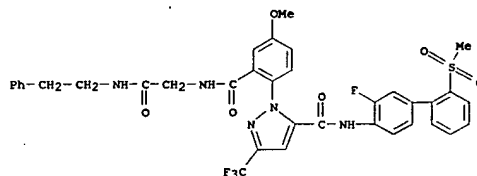
RN 885022-73-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[(1S)-4-amino-1-[(2-phenylethyl)amino]carbonyl]butyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

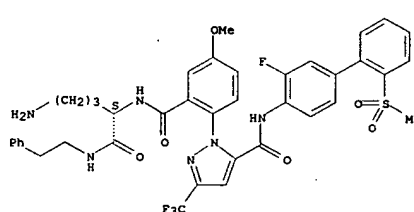


RN 885022-69-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
 4-yl]-1-[4-methoxy-2-[[[3-oxo-2-[(2-phenylethyl)amino]ethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



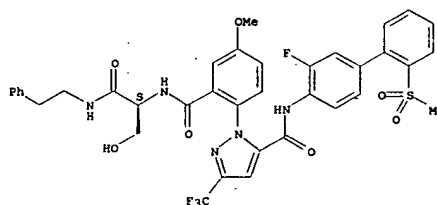
RN 885022-70-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
 4-yl]-1-[4-methoxy-2-[[[3-oxo-3-[(2-phenylethyl)amino]propyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-74-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
 4-yl]-1-[2-[[[(1S)-1-[(hydroxymethyl)-2-oxo-2-[(2-phenylethyl)amino]ethyl]amino]carbonyl]-4-methoxyphenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

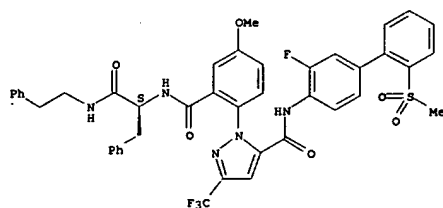
Absolute stereochemistry.



RN 885022-75-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
 4-yl]-1-[4-methoxy-2-[[[(1S)-2-oxo-2-[(2-phenylethyl)amino]ethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

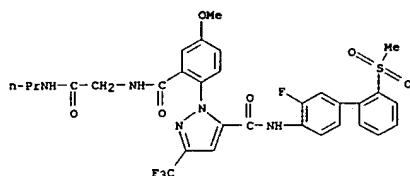
Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-76-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)][1,1'-biphenyl]-

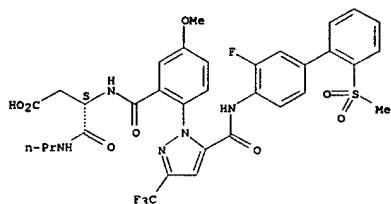
4-yl]-1-[4-methoxy-2-[[[2-oxo-2-(propylamino)ethyl]amino]carbonyl]phenyl]-
3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 885022-77-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)][1,1'-biphenyl]-

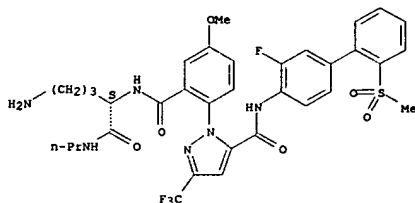
4-yl]-1-[4-methoxy-2-[[[3-oxo-3-(propylamino)propyl]amino]carbonyl]phenyl]-
3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-81-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[1S]-4-amino-1-
((propylamino)carbonyl)butyl]amino]carbonyl]-4-methoxyphenyl]-N-[3-fluoro-
2'-(methylsulfonyl)][1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

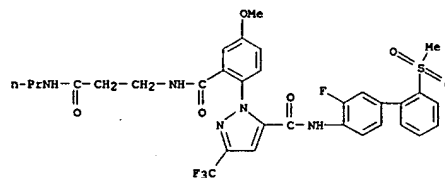


RN 885022-82-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)][1,1'-biphenyl]-

4-yl]-1-[2-[[[1S]-1-(hydroxymethyl)-2-oxo-2-(propylamino)ethyl]amino]carbonyl]-4-methoxyphenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

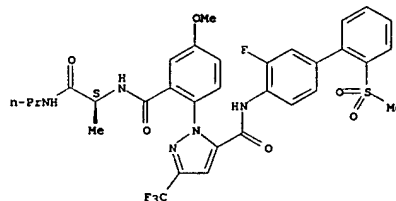
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 885022-79-7 CAPLUS

CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)][1,1'-biphenyl]-
4-yl]-1-[4-methoxy-2-[[[1S]-1-methyl-2-oxo-2-
(propylamino)ethyl]amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

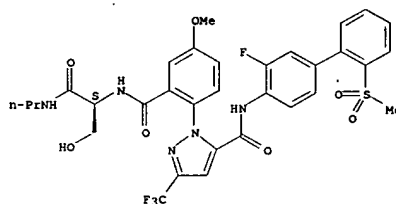


RN 885022-80-0 CAPLUS

CN Butanoic acid, 3-[[2-[5-[[[3-fluoro-2'-(methylsulfonyl)][1,1'-biphenyl]-4-
yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]-5-
methoxybenzoyl]amino]-4-oxo-4-(propylamino)-, (3S)- (9CI) (CA INDEX
NAME)

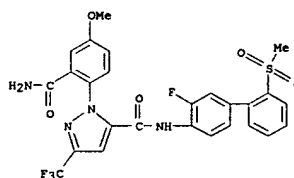
Absolute stereochemistry.

L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



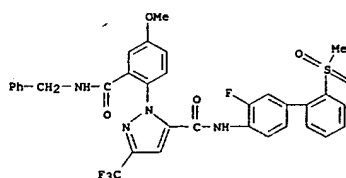
RN 885022-83-3 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminocarbonyl)-4-methoxyphenyl]-N-[3-
fluoro-2'-(methylsulfonyl)][1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-
(9CI) (CA INDEX NAME)



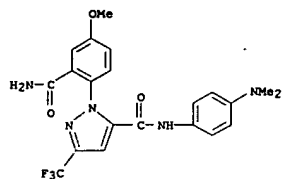
RN 885022-84-4 CAPLUS

CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)][1,1'-biphenyl]-
4-yl]-1-[4-methoxy-2-[[[phenylmethyl]amino]carbonyl]phenyl]-3-
(trifluoromethyl)- (9CI) (CA INDEX NAME)



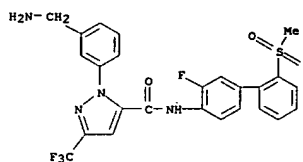
L9 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 985022-97-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminocarbonyl)-4-methoxyphenyl]-N-[4-(dimethylamino)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 5 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:188866 CAPLUS
 DOCUMENT NUMBER: 144:362579
 TITLE: Aminobenzisoxazoles with biaryl P4 moieties as potent, selective, and orally bioavailable factor Xa inhibitors
 AUTHOR(S): Quan, Mimi L.; Han, Qi; Fevig, John M.; Lam, Patrick Y. S.; Bai, Steve; Knabb, Robert M.; Luetttgen, Joseph M.; Wong, Pancras C.; Wexler, Ruth R.
 CORPORATE SOURCE: Discovery Chemistry, Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ, 08543, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(7), 1795-1798
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 144:362579
 AB We have previously reported on a series of aminobenzisoxazoles as potent, selective, and orally bioavailable factor Xa inhibitors, which culminated in the discovery of razaxaban. Herein, we describe another approach to improve factor Xa inhibitory potency and pharmacokinetic profile by incorporating basic and water soluble functionalities on the terminal ring of the P4 biaryl group found in our earlier Xa inhibitors. This approach resulted in a series of potent, selective, and orally bioavailable factor Xa inhibitors.
 IT 292135-59-2, DPC423
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (Aminobenzisoxazoles with biaryl P4 moieties as potent, selective, and orally bioavailable factor Xa inhibitors)
 RN 292135-59-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

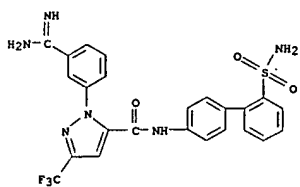
L9 ANSWER 5 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

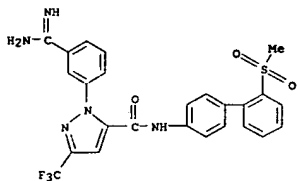
L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:165187 CAPLUS
 DOCUMENT NUMBER: 144:304521
 TITLE: Comparative study of factor Xa inhibitors using molecular docking/SVM/HQSAR/3D-QSAR methods
 AUTHOR(S): Sun, Jing; Chen, Hai Feng; Xia, Hai Rong; Yao, Jian Hua; Fan, Bo Tao
 CORPORATE SOURCE: Laboratory of Computer Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
 SOURCE: QSAR & Combinatorial Science (2006), 25(1), 25-45
 CODEN: QCSSAU; ISSN: 1611-020X
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The binding modes of a group of Factor Xa (fXa) inhibitors were studied using FlexX, CoMFA, CoMSIA, HQSAR and SVM models for inhibition potency were constructed with the conformers obtained from the mol. docking. 3D-QSAR models for oral bioavailability were also constructed with the subset inhibitors. The results show that these models possess good prediction ability. The influence of substituents for the activity and oral bioavailability were explored by comparing the constructed 3D-QSAR models. We found that some substituents have consistent effects on inhibition potency and oral bioavailability, but some have inconsistent effects. We observed equally that the different methods involved in this study, such as mol. docking, SVM, HQSAR and 3D-QSAR models, could be used not only for the prediction, but they are also complementary each to other. They are helpful for better understanding the interaction mechanism between inhibitors and fXa receptor.
 IT 209954-59-6 209954-94-9 209955-38-4
 209955-48-6 209955-60-2 209957-33-5
 209957-35-7 209957-47-1 228257-38-3
 228257-44-1 228257-50-9 228257-56-5
 228258-43-3 228258-44-4 228258-45-5
 228258-46-6 875139-46-1 875139-51-8
 875139-66-5 875139-67-6
 RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (comparative study of factor Xa inhibitors using mol. docking/SVM/HQSAR/QSAR methods)
 RN 209954-59-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

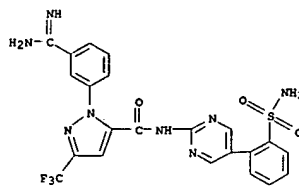


RN 209954-94-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

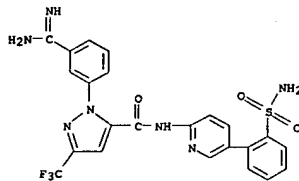


RN 209955-38-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

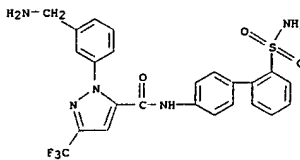


RN 209955-48-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

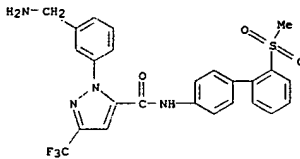


RN 209955-60-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

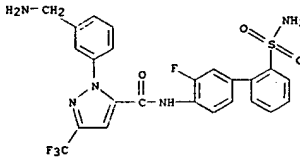
L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209957-33-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

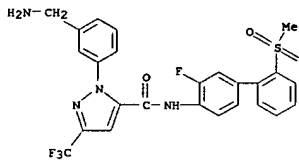


RN 209957-35-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

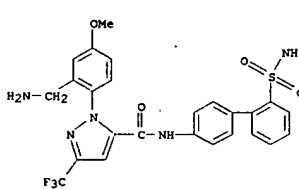


RN 209957-47-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

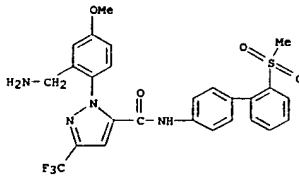
L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228257-38-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

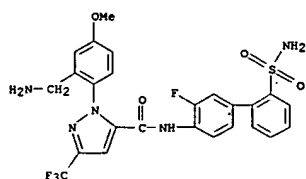


RN 228257-44-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

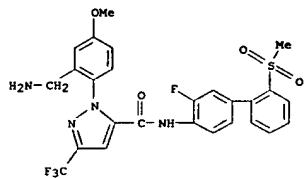


RN 228257-50-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

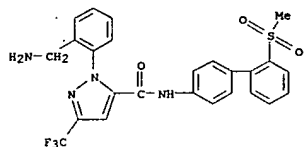
L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



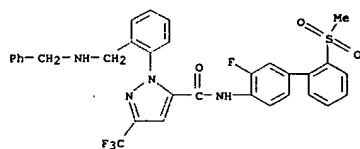
RN 228257-56-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



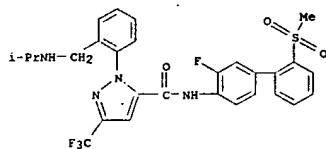
RN 228258-43-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



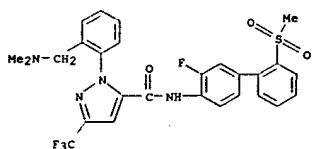
L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 RN 875139-46-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[2-[(phenylmethyl)amino]methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 875139-51-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[2-[(1-methylethyl)amino]methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



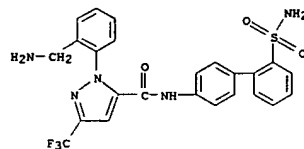
RN 875139-66-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-[(dimethylamino)methyl]phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



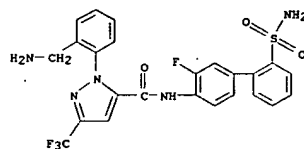
RN 875139-67-6 CAPLUS

10519356a.trn

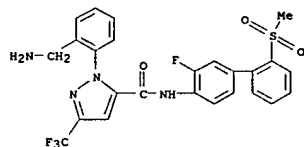
L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 RN 228258-44-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



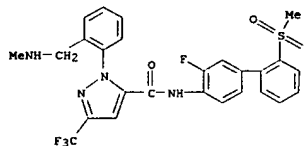
RN 228258-45-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 228258-46-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 RN 875139-46-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L9 ANSWER 7 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1021642 CAPLUS
DOCUMENT NUMBER: 143:311996
TITLE: Methods for inhibiting platelet activation and aggregation, and therapeutic uses for conditions or surgical procedures that may result in unwanted platelet aggregation
INVENTOR(S): Porter, Stephen R.; Flaharty, Kristen K.; Tcheng, James E.; Ferkany, John W.
PATENT ASSIGNEE(S): Vvdi Pharmaceuticals, USA
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXKX2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005087266	A1	20050922	WO 2005-US7440	20050307
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LA, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SH, TD, TG			

PRIORITY APPLN. INFO.: US 2004-550792P P 20040305

AB The invention features methods for preventing platelet activation and aggregation and for treating individuals suffering from conditions or undergoing procedures that may result in unwanted platelet aggregation. The methods are based on the i.v., s.c., or transdermal administration of a platelet activation or aggregation inhibitor, e.g., xemilofiban, followed by oral administration of the same or a different platelet activation or aggregation inhibitor. The treatment may commence prior to a medical or surgical procedure or after the outbreak of an adverse medical condition, either of which results in the activation of platelets that may lead to thrombus formation, and may continue thereafter.

IT 292135-59-2, DPC423
RL: AMT (Analyte); ANST (Analytical study)
(combination therapy for inhibition of platelet aggregation)

RN 292135-59-2 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-(3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl)-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 8 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:777848 CAPLUS
DOCUMENT NUMBER: 145:262418
TITLE: A Critical Assessment of Docking Programs and Scoring Functions
AUTHOR(S): Warren, Gregory L.; Andrews, C. Webster; Capelli, Anna-Maria; Clarke, Brian; LaLonde, Judith; Lambert, Millard H.; Lindvall, Mika; Nevins, Neysa; Semus, Simon F.; Senger, Stefan; Tedesco, Giovanna; Wall, Ian
CORPORATE SOURCE: D.; Woolven, James M.; Peishoff, Catherine E.; Head, Martha S.
GlaxoSmithKline Pharmaceuticals, Collegeville, PA, 19426, USA
SOURCE: Journal of Medicinal Chemistry (2006), 49(20), 5912-5931
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

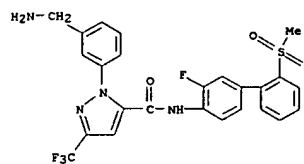
AB Docking is a computational technique that samples conformations of small mols. in protein binding sites; scoring functions are used to assess which of these conformations best complements the protein binding site. An evaluation of 10 docking programs and 37 scoring functions was conducted against eight proteins of seven protein types for three tasks: binding mode prediction, virtual screening for lead identification, and rank-ordering by affinity for lead optimization. All of the docking programs were able to generate ligand conformations similar to crystallog. determined protein/ligand complex structures for at least one of the targets. However, scoring functions were less successful at distinguishing the crystallog. conformation from the set of docked poses. Docking programs identified active compds. from a pharmaceutically relevant pool of decoy compds.; however, no single program performed well for all of the targets. For prediction of compound affinity, none of the docking programs or scoring functions made a useful prediction of ligand binding affinity.

IT 209957-47-1
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(critical assessment of docking programs and scoring functions)

RN 209957-47-1 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-(3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 7 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

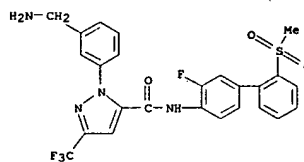


● HCl

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L9 ANSWER 8 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L9 ANSWER 9 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:511199 CAPLUS
 DOCUMENT NUMBER: 143:145801
 TITLE: Ligand-based assessment of factor Xa binding site flexibility via elaborate pharmacophore exploration and genetic algorithm-based QSAR modeling
 AUTHOR(S): Taha, Mutaseem O.; Qandil, Amjad M.; Zaki, Dhaia D.; Aldamen, Murad A.
 CORPORATE SOURCE: Faculty of Pharmacy, Department of Pharmaceutical Sciences, University of Jordan, Amman, Jordan
 SOURCE: European Journal of Medicinal Chemistry (2005), 40(7),

701-727
 CODEN: EJMCA5; ISSN: 0223-5234
 PUBLISHER: Elsevier Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The flexibility of activated factor X (fXa) binding site was assessed employing ligand-based pharmacophore modeling combined with genetic algorithm (GA)-based QSAR modeling. Four training subsets of wide structural diversity were selected from a total of 199 direct fXa inhibitors and were employed to generate different fXa pharmacophoric hypotheses using CATALYST software over two subsequent stages. In the first stage, high quality binding models (hypotheses) were identified. However, in the second stage, these models were refined by applying variable feature weight anal. to assess the relative significance of

their features in the ligand-target affinity. The binding models were validated according to their coverage (capacity as a three-dimensional (3D)

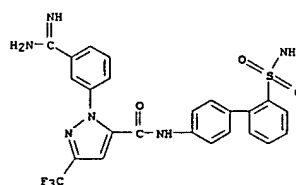
database search queries) and predictive potential as three-dimensional quant. structure-activity relationship (3D-QSAR) models. Subsequently, GA and multiple linear regression (MLR) anal. were employed to construct different QSAR models from high quality pharmacophores and explore the statistical significance of combination models in explaining bioactivity variations across 199 fXa inhibitors. Three orthogonal pharmacophoric models emerged in the optimal QSAR equation suggesting they represent three binding modes accessible to ligands in the binding pocket within fXa.

IT 209954-59-6 209955-48-6 209955-60-2
 209957-35-7 209957-47-1 209957-51-7
 209957-53-9

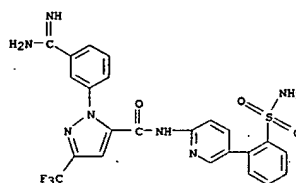
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (ligand-based assessment of factor Xa binding site flexibility via elaborate pharmacophore exploration and genetic algorithm-based QSAR modeling)

RN 209954-59-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 9 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

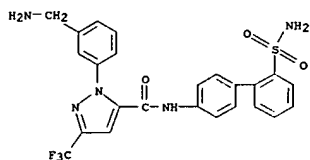


RN 209955-48-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

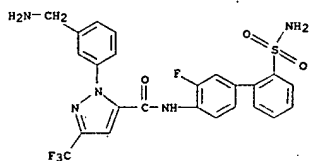


RN 209955-60-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

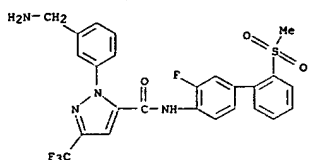
L9 ANSWER 9 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209957-35-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

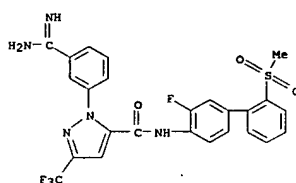


RN 209957-47-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

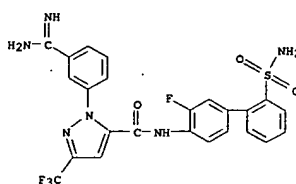


RN 209957-51-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 9 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209957-53-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 85 THERE ARE 85 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L9 ANSWER 10 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:1151496 CAPLUS
 DOCUMENT NUMBER: 142:328858
 TITLE: The chimpanzee (Pan troglodytes) as a pharmacokinetic model for selection of drug candidates: Model characterization and application
 AUTHOR(S): Wong, Harvey; Grossman, Scott J.; Bai, Stephen A.; Diamond, Sharon; Wright, Matthew R.; Grace, James E., Jr.; Qian, Mingxin; He, Kan; Yeleswaram, Krishnaaswamy; Christ, David D.
 CORPORATE SOURCE: Metabolism and Pharmacokinetics, Bristol-Myers Squibb Company, Wallingford, CT, USA
 SOURCE: Drug Metabolism and Disposition (2004), 32(12), 1359-1369
 CODEN: DMDSDI; ISSN: 0090-9556
 PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The chimpanzee (CHP) was evaluated as a pharmacokinetic model for humans (HUMs) using propranolol, verapamil, theophylline, and 12 proprietary compds. Species differences were observed in the systemic clearance of theophylline (.apprx.5-fold higher in CHPs), a low clearance compound, and the bioavailability of propranolol and verapamil (lower in CHPs), both high clearance compds. The systemic clearance of propranolol (.apprx.1.53 l/h/kg) suggested that the hepatic blood flow in CHPs is comparable to that in humans. No substantial differences were observed in the in vitro protein binding. A preliminary attempt was made to characterize cytochrome P 450 activities in CHP and HUM liver microsomes.
 Testosterone 6 β -hydroxylation and tolbutamide methylhydroxylation activities were comparable in CHP and HUM liver microsomes. In contrast, dextromethorphan O-demethylation and phenacetin O-deethylation activities were .apprx.10-fold higher (per mg protein) in CHP liver microsomes.
 Intrinsic clearance ests. in CHP liver microsomes were higher for propranolol (.apprx.10-fold) and theophylline (.apprx.5-fold) and similar for verapamil. Of the 12 proprietary compds., 3 had oral clearances that differed in the two species by more than 3-fold, an acceptable range for biol. variability. Most of the observed differences are consistent with species differences in P 450 enzyme activity. Oral clearances of proprietary compds. in HUMs were significantly correlated to those from CHPs ($r = 0.68$; $p = 0.015$), but not to ests. from rat, dog, and monkey. In summary, the chimpanzee serves as a valuable surrogate model for human pharmacokinetics, especially when species differences in P 450 enzyme activity are considered.
 IT 292135-59-2, DPC 423
 RL: PKT (Pharmacokinetics); BIOL (Biological study) (chimpanzee (Pan troglodytes) as a surrogate model for human pharmacokinetic studies in relation to species differences in P 450 enzyme activity)

L9 ANSWER 11 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:799558 CAPLUS
 DOCUMENT NUMBER: 141:296012
 TITLE: Preparation of factor Xa- and thrombin-inhibiting substituted benzamides and sulfonylbenzamides as potential anticoagulants
 INVENTOR(S): Pinto, Donald J.; Qiao, Jennifer X.; Gangor, Timur; Lam, Patrick Y. S.; Li, Yun-long
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
 SOURCE: PCT Int. Appl., 279 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004083174	A2	20040930	WO 2004-US8033	20040317
WO 2004083174	A3	20041125		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BU, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZH, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2004209863	A1	20041021	US 2004-801518	20040316
US 7122557	B2	20061017		
EP 1603562	A2	20051214	EP 2004-757516	20040317
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK			
PRIORITY APPLN. INFO.:			US 2003-455709P	P 20030318
			US 2004-801518	A 20040316
			WO 2004-US8033	W 20040317

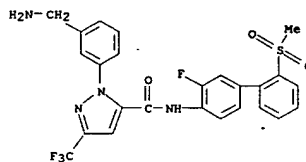
OTHER SOURCE(S): HARPAT 141:296012
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. P4-M-M4 (I) [M = (un)substituted 3-10 membered carbocyclic or a 4-10 membered heterocyclic ring containing 1-3 O, N, or S atoms, alone or fused to an (un)substituted 5-7 membered carbocycle or heterocycle; P4 = Z-A-B; M4 = G-G1; A = (un)substituted 3-10 membered carbocyclic or 5-12 membered heterocyclic ring; B = (un)substituted amidino, guanidino, iminomethyl; G = five or six-membered carbocycle or heterocycle fused to benzene, pyridine, pyrimidine, pyrazine, or pyridazine ring; G1 = bond, (un)substituted alkyl, alkenyl, alkynyl; Z = (un)substituted alkylene], such as tetrahydropyrazolo[3,4-c]pyridinone II or

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L9 ANSWER 10 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 RN 292135-59-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



• HCl

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

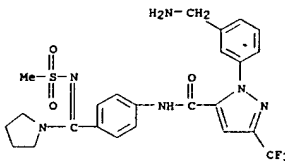
L9 ANSWER 11 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 (pyridinylaminocarbonylphenylaminocarbonyl)benzamide III are prepd. as inhibitors of Factor Xa and thrombin for use as anticoagulants. Deprotonation of 2-amino-4-chloropyridine and addn. to 5-chloroisatoic anhydride yields N-(5-chloro-2-pyridinyl) 2-amino-5-chlorobenzamide (IV). Acid-mediated addn. of dimethylamine to the nitrile of Me 4-cyanobenzoate, mesylation of the amidine nitrogen, and base-mediated hydrolysis of the ester yields 4-(N,N-dimethyl-N'-methylsulfonylamidino)benzoic acid (V). Coupling of IV and V mediated by BOP yields III. Some compds. of the invention inhibit human factor Xa with Ki values of ≤ 10 nM; in addn., some of the invention compds. inhibit thrombin in vitro. (no data).
 IT 764658-97-1P 764658-98-2P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of factor Xa- and thrombin-inhibiting substituted benzamides and sulfonylbenzamides as potential anticoagulants)

RN 764658-97-1 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-

[(methylsulfonyl)imino]-1-pyrrolidinylmethyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

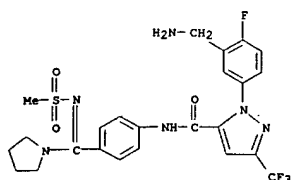


RN 764658-98-2 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[4-

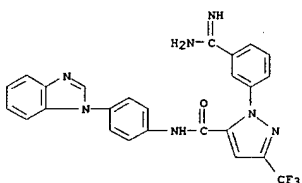
[(methylsulfonyl)imino]-1-pyrrolidinylmethyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 11 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:791919 CAPLUS
 DOCUMENT NUMBER: 141:342889
 TITLE: SAR and factor IXa crystal structure of a dual inhibitor of factors IXa and Xa
 AUTHOR(S): Smallheer, Joanne M.; Alexander, Richard S.; Wang, Jianmin; Wang, Shuaige; Nakajima, Suanne; Rossi, Karen
 A.: Smallwood, Angela; Barbera, Frank; Burdick, Debra;
 Luetgten, Joseph M.; Knabb, Robert M.; Wexler, Ruth R.; Jadhav, Prabhakar K.
 CORPORATE SOURCE: Bristol-Myers Squibb Company, Princeton, NJ, 08543-5400, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(21), 5263-5267
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:342889
 AB Modifications to the P4 moiety and pyrazole C3 substituent of factor Xa inhibitor SN-429 provided several new compds., which are 5-10 nM inhibitors of factor IXa. An x-ray crystal structure of one example complexed to factor IXa shows that these compds. adopt a similar binding mode to that previously observed with pyrazole inhibitors in the factor Xa active site both with regard to how the inhibitor binds and the position of Tyr99.
 IT 848393-61-3P 848393-63-5P 848393-64-6P
 848393-85-1P 848393-86-2P 848393-88-4P
 848393-89-5P 848393-91-1P 848393-92-0P
 848393-93-1P 848393-95-3P 848393-96-4P
 848393-97-5P 848393-98-6P 848393-99-7P
 848394-00-3P
 RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (pyrazole compds. preparation, crystal structure, and dual inhibition of factors IXa and Xa)
 RN 848393-61-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)
 CH 1
 CRN 774218-45-0
 CMF C25 H18 F3 N7 O

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

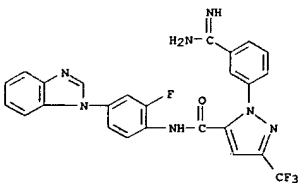


CH 2
 CRN 76-05-1
 CMF C2 H F3 O2



RN 848393-63-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CH 1
 CRN 774218-46-1
 CMF C25 H17 F4 N7 O



CH 2

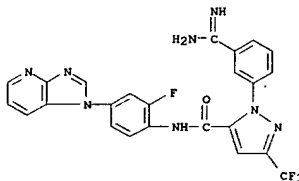
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L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 848393-64-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(1H-imidazo[4,5-b]pyridin-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CH 1
 CRN 774218-47-2
 CMF C24 H16 F4 N8 O



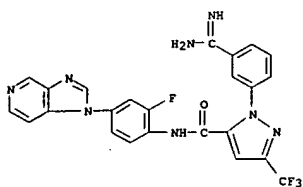
CH 2
 CRN 76-05-1
 CMF C2 H F3 O2



RN 848393-85-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(1H-imidazo[4,5-c]pyridin-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CH 1
 CRN 774218-48-3

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CHF C24 H16 F4 N8 O



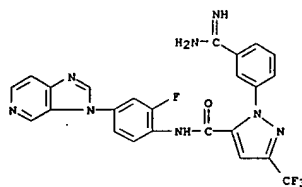
CH 2
CRN 76-05-1
CHF C2 H F3 O2



RN 848393-86-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(3H-imidazo[4,5-c]pyridin-3-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CH 1
CRN 774218-49-4
CHF C24 H16 F4 N8 O

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

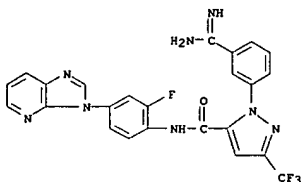


CH 2
CRN 76-05-1
CHF C2 H F3 O2



RN 848393-88-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(3H-imidazo[4,5-b]pyridin-3-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CH 1
CRN 774218-50-7
CHF C24 H16 F4 N8 O



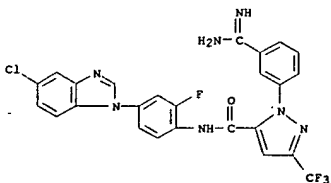
L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CH 2
CRN 76-05-1
CHF C2 H F3 O2



RN 848393-89-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5-chloro-1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CH 1
CRN 774218-51-8
CHF C25 H16 Cl F4 N7 O



CH 2
CRN 76-05-1
CHF C2 H F3 O2

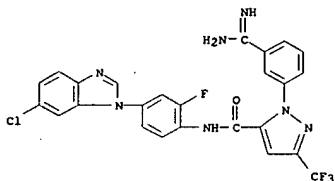


RN 848393-91-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(6-chloro-1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

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L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CH 1
CRN 774218-52-9
CHF C25 H16 Cl F4 N7 O



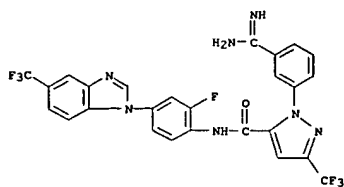
CH 2
CRN 76-05-1
CHF C2 H F3 O2



RN 848393-92-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(5-(trifluoromethyl)-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CH 1
CRN 774218-53-0
CHF C26 H16 F7 N7 O

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2
CRN 76-05-1
CMF C2 H F3 O2



RN 848393-93-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(5-
methyl-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)-,
trifluoroacetate (9CI) (CA INDEX NAME)

CM 1
CRN 774218-54-1
CMF C26 H19 F4 N7 O

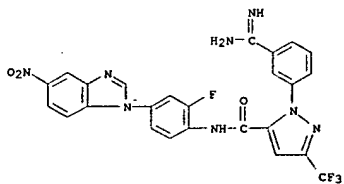
L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 2
CRN 76-05-1
CMF C2 H F3 O2



RN 848393-96-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(5-
nitro-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate
(9CI) (CA INDEX NAME)

CM 1
CRN 774218-56-3
CMF C25 H16 F4 N8 O3



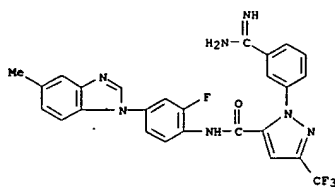
CM 2
CRN 76-05-1
CMF C2 H F3 O2



RN 848393-97-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5,6-
dichloro-1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-,

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L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

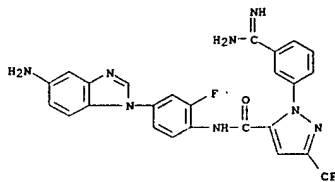


CM 2
CRN 76-05-1
CMF C2 H F3 O2



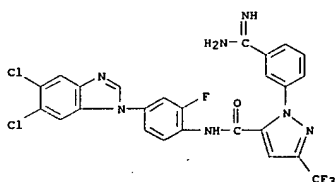
RN 848393-95-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[4-(5-amino-1H-benzimidazol-1-yl)-2-
fluorophenyl]-1-[3-(aminoiminomethyl)phenyl]-3-(trifluoromethyl)-,
trifluoroacetate (9CI) (CA INDEX NAME)

CM 1
CRN 774218-55-2
CMF C25 H18 F4 N8 O



L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1
CRN 774218-57-4
CMF C25 H15 Cl2 F4 N7 O



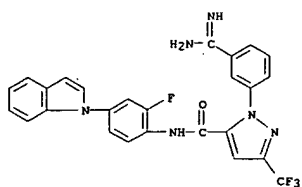
CM 2
CRN 76-05-1
CMF C2 H F3 O2



RN 848393-98-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-
(1H-indol-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA
INDEX NAME)

CM 1
CRN 774218-58-5
CMF C26 H18 F4 N6 O

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

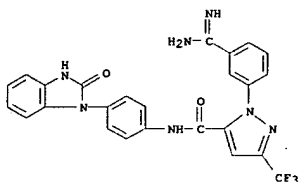


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 CRN 76-05-1
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RN 848393-99-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

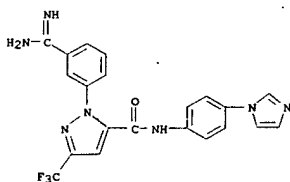
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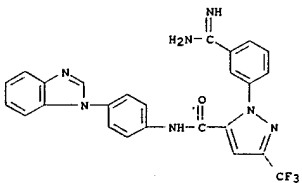
L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 209956-75-2P 774218-45-0P 774218-46-1P
 774218-47-2P 774218-48-3P 774218-49-4P
 774218-50-7P 774218-51-8P 774218-52-9P
 774218-53-0P 774218-54-1P 774218-55-2P
 774218-56-3P 774218-57-4P 774218-58-5P
 774218-59-6P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (pyrazole compds. preparation, crystal structure, and dual inhibition

of factors IXa and Xa)
 RN 209956-75-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 774218-45-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 774218-46-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

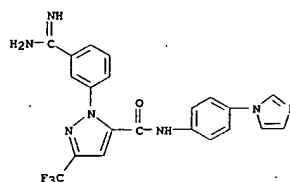
L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 2
 CRN 76-05-1
 CMF C2 H F3 O2



RN 848394-00-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

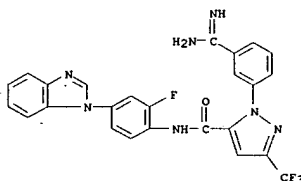
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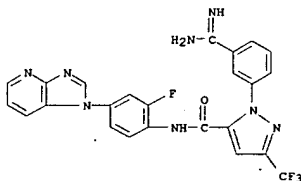
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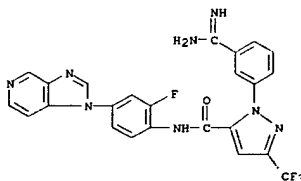
L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 774218-47-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(1H-imidazo[4,5-b]pyridin-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

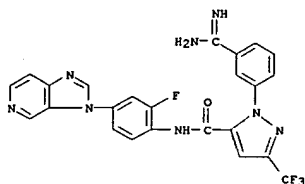


RN 774218-48-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(1H-imidazo[4,5-c]pyridin-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

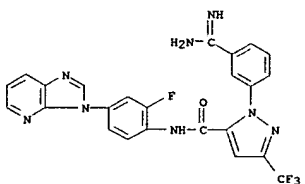


RN 774218-49-4 CAPLUS

L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(3H-imidazo[4,5-c]pyridin-3-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



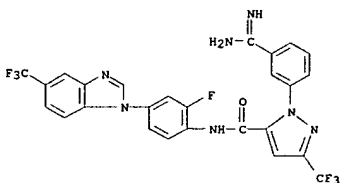
RN 774218-50-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(3H-imidazo[4,5-b]pyridin-3-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



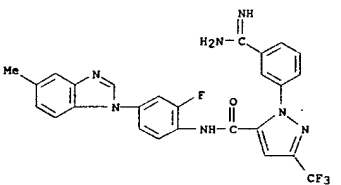
RN 774218-51-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5-chloro-1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



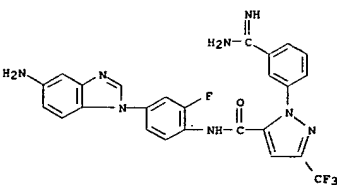
L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



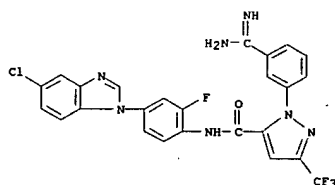
RN 774218-54-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(5-methyl-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



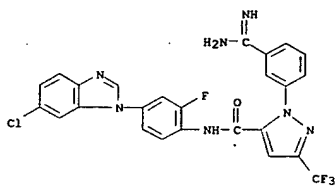
RN 774218-55-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[4-(5-amino-1H-benzimidazol-1-yl)-2-fluorophenyl]-1-[3-(aminoiminomethyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



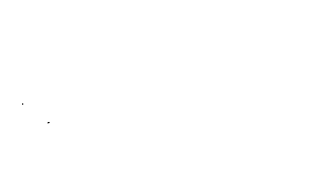
L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 774218-52-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(6-chloro-1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

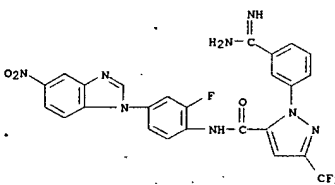


RN 774218-53-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(5-(trifluoromethyl)-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

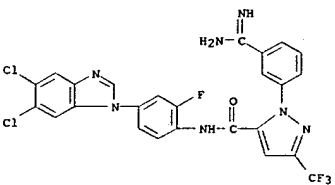


L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 774218-56-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(5-nitro-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



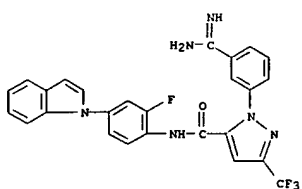
RN 774218-57-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5,6-dichloro-1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



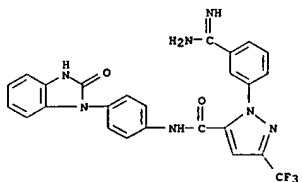
RN 774218-58-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2-fluoro-4-(1H-indol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

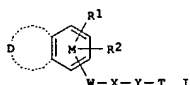


RN 774218-59-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI)
 (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB Title compds. [I: D = (N-, O-, S-interrupted) (substituted) C3-4 alkylene;
 M = Ph, aromatic heterocyclyl; R1, R2 = H, halo, (branched) (interrupted) (substituted) alkyl, NO2, cyano, OR3, N(R3)2, CO2R3, CON(R3)2, C(S)N(R3)2, etc.; R3 = H, (branched) (interrupted) (substituted) alkyl, etc.; W = (substituted) (bi)cyclic aromatic (hetero)cyclyl; X = CONR3, CONR3C(R4)2, C(R4)2NR3, etc.; R4 = H, (branched) (interrupted) (substituted) alkyl; Y = alkylene, cycloalkylene, heterodiy, aryldiy; T = (substituted) (bi)cyclic aromatic heterocyclyl, were prepared Thus, 333 mg

(3-[5-(4-(2-iminopyrrolidin-1-yl)phenyl)carbamoyl]-3-trifluoromethylpyrazol-1-yl)benzyl)carbamoyl acid tert-Bu ester (preparation given) in EtOH was treated

with HCl in ether to give 289 mg

N-[4-(2-iminopyrrolidin-1-yl)phenyl]-1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide. The latter gave affinity to the receptor Xa with IC50 = 9,6·10⁻⁹ M and to the receptor VIIa with IC50 = 2,3·10⁻⁸ M.

IT 640287-97-4P 640288-03-5P 640288-05-7P
 640288-06-8P 640288-07-9P 640288-11-5P
 640288-12-6P 640288-13-7P 640288-20-6P
 640288-21-7P 640288-22-8P 640288-23-9P
 640288-24-0P 640288-25-1P 640288-26-2P
 640288-27-3P 640288-28-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (thioxoheterocyclyl)phenyl) (phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

RN 640287-97-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)-, dihydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:20490 CAPLUS

DOCUMENT NUMBER: 140:77148

TITLE: Preparation of N-[4-(thioxoheterocyclyl)phenyl]-2-phenyl-2H-pyrazole-3-carboxamides and corresponding imino-heterocyclyl derivatives as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis

INVENTOR(S): Cezanne, Bertram; Dorsch, Dieter; Mederski, Werner; Tsaklakidis, Christos; Gleitz, Johannes; Barnes, Christopher

PATENT ASSIGNEE(S): Merck Patent GmbH, Germany

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PTKDZ

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

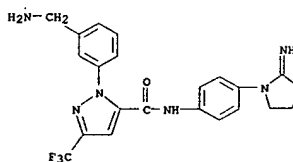
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004002477	A1	20040108	WO 2003-EP5898	20030605
WO 2004002477	A8	20040415		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GR, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, NE, SD, SI, SE, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
DE 10229070	A1	20040115	DE 2002-10229070	20020628
CA 2491271	A1	20040108	CA 2003-2491271	20030605
AU 2003238475	A1	20040119	AU 2003-238475	20030605
EP 1517685	A1	20050330	EP 2003-732540	20030605
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
JP 2005535630	T	20051124	JP 2004-516575	20030605
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US 2005203127	A1	20050915	US 2004-519356	20041228
PRIORITY APPLN. INFO.:			DE 2002-10229070	A 20020628
			EP 2003-732540	A3 20030605
			WO 2003-EP5898	W 20030605

OTHER SOURCE(S): MARPAT 140:77148

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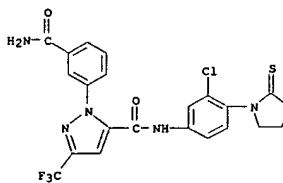
L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● 2 HCl

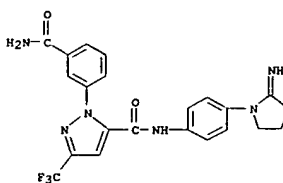
RN 640288-03-5 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-chloro-4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



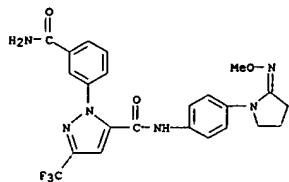
RN 640288-05-7 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

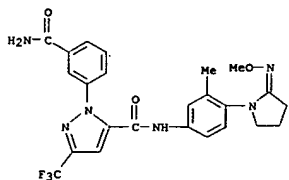


RN 640288-06-8 CAPLUS

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-methoxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

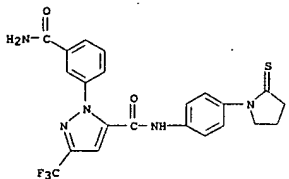


RN 640288-07-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-methoxyimino)-1-pyrrolidinyl]-3-methylphenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

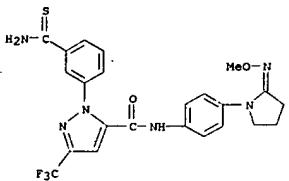


RN 640288-11-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[3-bromo-4-(2-imino-5-methyl-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

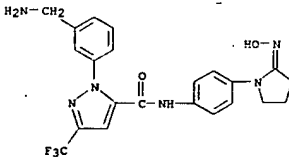
L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 640288-20-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminothioxomethyl)phenyl]-N-[4-(2-methoxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

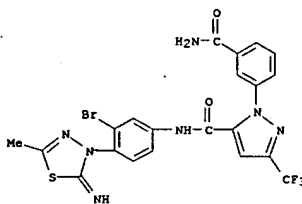


RN 640288-21-7 CAPLUS
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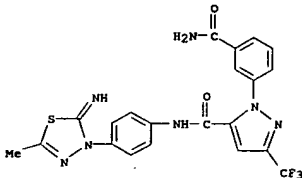


RN 640288-22-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-amino-4,5-dihydro-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

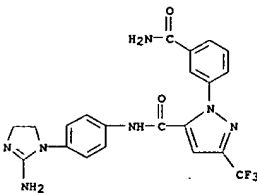


RN 640288-12-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-imino-5-methyl-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

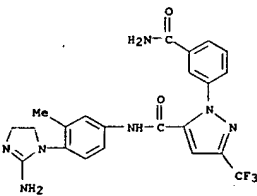


RN 640288-13-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

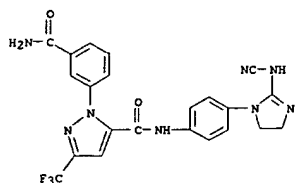


RN 640288-23-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-amino-4,5-dihydro-1H-imidazol-1-yl)-3-methylphenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

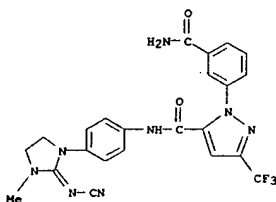


RN 640288-24-0 CAPLUS
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L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

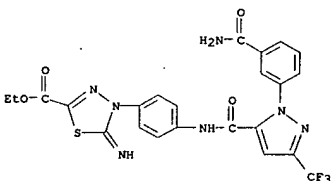


RN 640288-25-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-cyanoimino)-3-methyl-1-imidazolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

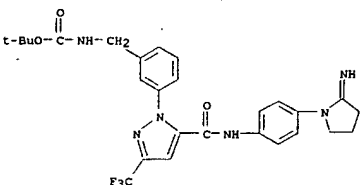


RN 640288-26-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(5-ethyl-2-imino-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



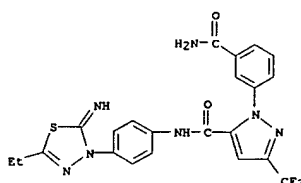
IT 640288-00-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of (thioxoheterocyclylphenyl) (phenylpyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)
RN 640288-00-2 CAPLUS
CN Carbamic acid, [[3-[5-[[[4-(2-imino-1-pyrrolidinyl)phenyl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



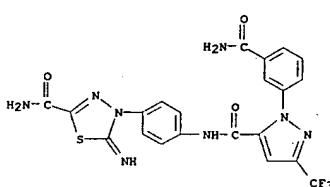
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RECORD

FORMAT

L9 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 640288-27-3 CAPLUS
CN 1,3,4-Thiadiazole-2-carboxamide, 4-[4-[[[1-[3-(aminocarbonyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-4,5-dihydro-5-imino- (9CI) (CA INDEX NAME)



RN 640288-28-4 CAPLUS
CN 1,3,4-Thiadiazole-2-carboxylic acid, 4-[4-[[[1-[3-(aminocarbonyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-4,5-dihydro-5-imino-, ethyl ester (9CI) (CA INDEX NAME)

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:644982 CAPLUS
DOCUMENT NUMBER: 140:59557
TITLE: Discovery of 1-(2-Aminomethylphenyl)-3-trifluoromethyl-N-[3-fluoro-2'-(aminosulfonyl)[1,1'-biphenyl]]-4-yl]-1H-pyrazole-5-carboxamide (DPC602), a Potent, Selective, and Orally Bioavailable Factor Xa Inhibitor

Inhibitor
AUTHOR(S): Pruitt, James R.; Pinto, Donald J. P.; Galembo, Robert
CORPORATE SOURCE: A., Jr.; Alexander, Richard S.; Rossi, Karen A.; Wells, Brian L.; Drummond, Spencer; Boström, Lori L.; Burdick, Debra; Bruckner, Robert; Chen, Haiying; Smallwood, Angela; Wong, Pancras C.; Wright, Matthew R.; Bai, Steven; Luetzgen, Joseph M.; Knabb, Robert M.; Lam, Patrick Y. S.; Wexler, Ruth R. Pharmaceutical Research Institute, Bristol-Myers Squibb Company, Pennington, NJ, 08534, USA
SOURCE: Journal of Medicinal Chemistry (2003), 46(25), 5298-5315
CODEN: JMCMAR; ISSN: 0022-2623

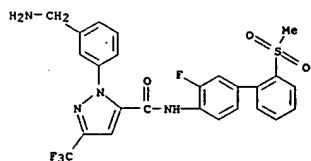
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:59557
AB Factor Xa, a serine protease, is at the critical juncture between the intrinsic and extrinsic pathways of the coagulation cascade. Inhibition of factor Xa has the potential to provide effective treatment for both venous and arterial thrombosis. The authors recently described a series of meta-substituted phenylpyrazoles that are highly potent, selective,

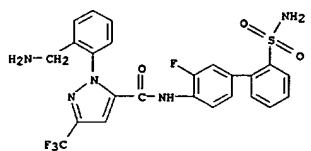
and orally bioavailable factor Xa inhibitors. In this paper, the authors report their efforts to further optimize the selectivity profile of the factor Xa inhibitors with a series of ortho- and/or para-substituted phenylpyrazole derivs. The most potent compds. display sub-nanomolar inhibition consts. for factor Xa and show greater than 1000-fold selectivity against other serine proteases. These compds. are also effective in a rabbit model of arteriovenous shunt thrombosis. Optimization of this series led to the preclin. development of DPC602, a 2-(aminomethyl)phenylpyrazole analog, as a highly potent, selective, and orally bioavailable factor Xa inhibitor.

IT 209957-47-1DP, factor Xa complex 228258-45-SDP, factor Xa complex
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure of)
RN 209957-47-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-45-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-
 3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



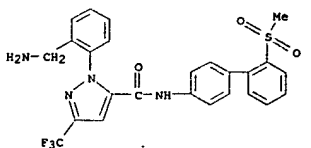
IT 228258-59-1P 228258-62-6P 228258-85-3P
 228258-86-4P 228258-87-5P 637318-67-3P
 637318-69-5P 637318-85-5P 637319-02-9P
 637319-13-2P 637319-15-4P 637319-17-6P
 637319-19-8P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
 (Biological study); PREP (Preparation)
 (preparation of
 1-(2-aminomethylphenyl)-3-trifluoromethyl-N-(3-fluoro-2'-
 (aminosulfonyl)[1,1'-biphenyl]-4-yl)-1H-pyrazole-5-carboxamide and
 related compds. as orally bioavailable factor Xa inhibitors)
 RN 228258-59-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-
 (aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)
 CH 1
 CRN 228257-50-9
 CHF C25 H21 F4 N5 O4 S

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CH 2
 CRN 76-05-1
 CHF C2 H F3 O2



RN 228258-85-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-
 (methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)
 CH 1
 CRN 228258-43-3
 CHF C25 H21 F3 N4 O3 S



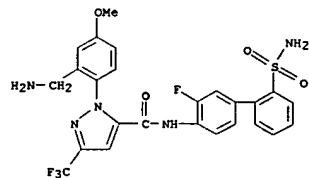
CH 2
 CRN 76-05-1
 CHF C2 H F3 O2



RN 228258-86-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-
 (aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)
 CH 1
 CRN 228258-44-4
 CHF C24 H20 F3 N5 O3 S

10519356a.trn

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

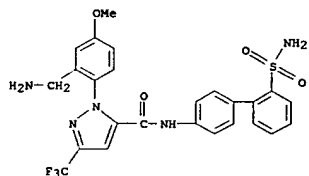


CH 2
 CRN 76-05-1
 CHF C2 H F3 O2

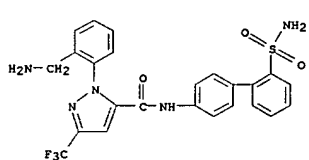


RN 228258-62-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-
 (aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
 CRN 228257-38-3
 CHF C25 H22 F3 N5 O4 S



L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

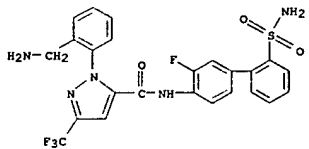


CH 2
 CRN 76-05-1
 CHF C2 H F3 O2



RN 228258-87-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-
 3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
 CRN 228258-45-5
 CHF C24 H19 F4 N5 O3 S



CH 2
 CRN 76-05-1
 CHF C2 H F3 O2

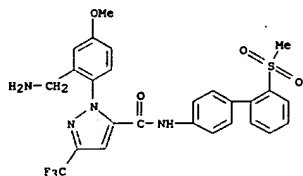
L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 637318-67-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, trifluoroacetate (10:13) (9CI) (CA INDEX NAME)

CH 1

CRN 228257-44-1
 CMF C26 H23 F3 N4 O4 S



CH 2

CRN 76-05-1
 CMF C2 H F3 O2



RN 637318-69-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, trifluoroacetate (2:3) (9CI) (CA INDEX NAME)

CH 1

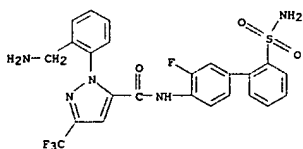
L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CH 2

CRN 76-05-1
 CMF C2 H F3 O2



RN 637319-02-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

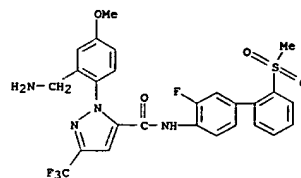
RN 637319-13-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 875139-67-6
 CMF C26 H22 F4 N4 O3 S

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 228257-56-5
 CMF C26 H22 F4 N4 O4 S



CH 2

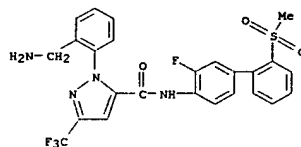
CRN 76-05-1
 CMF C2 H F3 O2



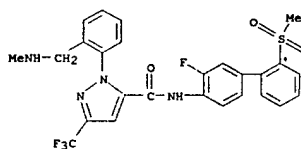
RN 637318-85-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, trifluoroacetate (10:11) (9CI) (CA INDEX NAME)

CH 1

CRN 228258-46-6
 CMF C25 H20 F4 N4 O3 S



L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CH 2

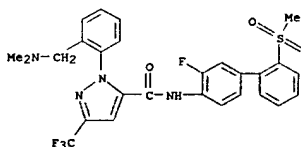
CRN 76-05-1
 CMF C2 H F3 O2



RN 637319-15-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-[(dimethylamino)methyl]phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 875139-66-5
 CMF C27 H24 F4 N4 O3 S



CH 2

CRN 76-05-1
 CMF C2 H F3 O2

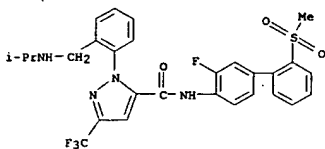
L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 637319-17-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
 4-yl]-1-[2-[[[(1-methylethyl)amino]methyl]phenyl]-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 875139-51-8
 CMF C28 H26 F4 N4 O3 S



CM 2

CRN 76-05-1
 CMF C2 H F3 O2

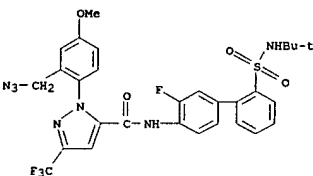


RN 637319-19-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
 4-yl]-1-[2-[[[(phenylmethyl)amino]methyl]phenyl]-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

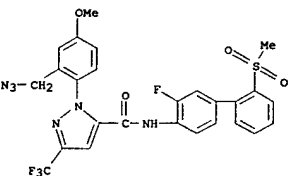
CM 1

CRN 875139-46-1

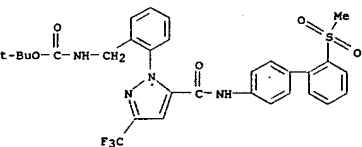
L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228259-22-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 1-[2-(azidomethyl)-4-methoxyphenyl]-N-[3-fluoro-
 2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
 INDEX NAME)



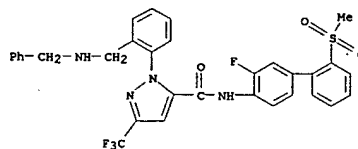
RN 228259-36-7 CAPLUS
 CN Carbamic acid, [[2-[5-[[[2'-(methylsulfonyl)[1,1'-biphenyl]-4-
 yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-,
 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 228259-37-8 CAPLUS
 CN Carbamic acid, [[2-[5-[[[2'-(methylsulfonyl)[1,1'-biphenyl]-4-
 yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-
 yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CMF C32 H26 F4 N4 O3 S



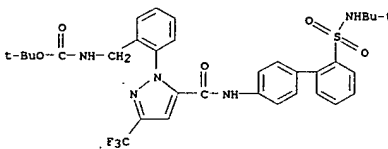
CM 2

CRN 76-05-1
 CMF C2 H F3 O2

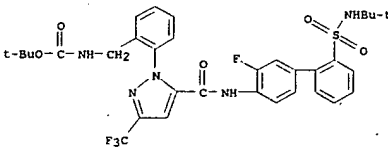


IT 228259-20-9P 228259-22-1P 228259-36-7P
 228259-37-8P 228259-38-9P 228259-39-0P
 637319-00-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of
 1-(2-aminomethylphenyl)-3-trifluoromethyl-N-[3-fluoro-2'-
 (aminosulfonyl)[1,1'-biphenyl]-4-yl]-1H-pyrazole-5-carboxamide and
 related compds. as orally bioavailable factor Xa inhibitors)
 RN 228259-20-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(azidomethyl)-4-methoxyphenyl]-N-[2'-
 [[[(1,1-dimethylethyl)amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]-3-
 (trifluoromethyl)- (9CI) (CA INDEX NAME)

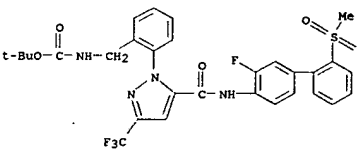
L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228259-38-9 CAPLUS
 CN Carbamic acid, [[2-[5-[[[2'-(methylsulfonyl)[1,1'-biphenyl]-4-
 fluoro[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-
 1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

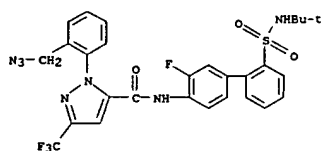


RN 228259-39-0 CAPLUS
 CN Carbamic acid, [[2-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-
 yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-,
 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 637319-00-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(azidomethyl)phenyl]-N-[2'-[[[(1,1-
 dimethylethyl)amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]-3-
 (trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT .

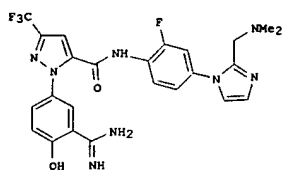
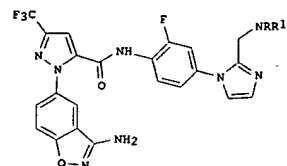
L9 ANSWER 15 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:454067 CAPLUS
 DOCUMENT NUMBER: 139:36524
 TITLE: Preparation of novel N-[4-(1H-imidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamides as factor Xa inhibitors
 INVENTOR(S): Quan, Mimi L.
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
 SOURCE: PCT Int. Appl., 66 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003047517	A2	20030612	WO 2002-US38168	20021126
WO 2003047517	A3	20040226		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GG, GW, ML, MR, NE, SN, TD, TG				
US 2003144287	B2	20040504	US 2002-302184	20021122
US 6730689	A1	20030617	AU 2002-352962	20021126
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EP 1460996	A2	20040929	EP 2002-789922	20021126
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HU 200402515	A2	20050329	HU 2004-2515	20021126
JP 2005527485	T	20050915	JP 2003-548778	20021126
PRIORITY APPLN. INFO.: US 2001-336972P P 20011204				
WO 2002-US38168 W. 20021126				

OTHER SOURCE(S): MARPAT 139:36524
 GI

L9 ANSWER 15 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB N-[4-(1H-imidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamides of formula I [R = H, alkyl; R1 = H, acyl, etc.] and derivs. thereof are prepared which are useful as inhibitors of factor Xa. Thus,

II was prepared in several steps. The prepared compds. had Ki values of ≤ 10 μM against human factor Xa.

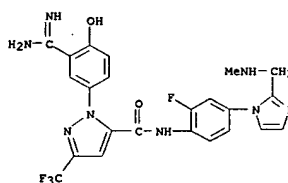
IT 540510-36-9P 540510-43-8P
 RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of imidazolylphenyl pyrazolecarboxamide derivs. as factor Xa inhibitors)

RN 540510-36-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)-4-hydroxyphenyl]-N-[2-fluoro-4-[2-[(methylamino)methyl]-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CH 1

CRN 540510-35-8
 CMF C23 H20 F4 N8 O2

L9 ANSWER 15 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

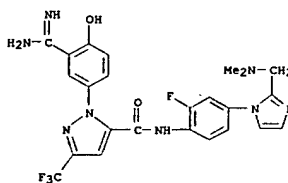


CH 2

CRN 76-05-1
 CMF C2 H F3 O2



RN 540510-43-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)-4-hydroxyphenyl]-N-[4-[2-[(dimethylamino)methyl]-1H-imidazol-1-yl]-2-fluorophenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

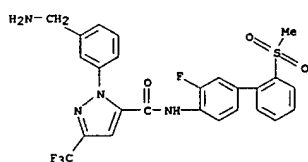


L9 ANSWER 16 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:363518 CAPLUS
 DOCUMENT NUMBER: 140:16
 TITLE: Factor Xa inhibitors: Today and beyond
 AUTHOR(S): Walenga, Jeanine M.; Jeske, Walter P.; Hoppensteadt, Debra; Fareed, Jawad
 CORPORATE SOURCE: Department of Pathology, Loyola University Medical Center, Maywood, IL, 60153, USA
 SOURCE: Current Opinion in Investigational Drugs (Thomson Current Drugs) (2003), 4(3), 272-281
 CODEN: COIDAZ; ISSN: 1472-4472
 PUBLISHER: Thomson Current Drugs
 DOCUMENT TYPE: Journal; General Review
 LANGUAGE: English

AB A review. Serine proteases play an important role in thrombogenesis, the process that leads to blood clotting and conditions such as heart attack, stroke and other cardiovascular disorders. In the coagulation network, the activation of various serine proteases facilitates the formation of the serine protease Factor Xa, which plays a central role in the process of coagulation and platelet activation. Factor Xa is an essential component of the prothrombinase complex, from which thrombin is formed, which then directly leads to fibrin clot formation. Thus, the inhibition of Factor Xa and its generation is an important strategy in the development of new antithrombotic drugs.

IT 292135-59-2, DPC-423
 RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (factor Xa inhibitors as antithrombotic drugs)

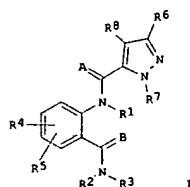
RN 292135-59-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 120 THERE ARE 120 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

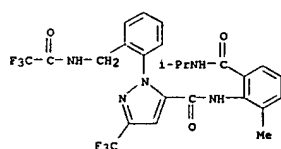
L9 ANSWER 17 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB An invertebrate pest control composition for coating a propagule comprises (1) a biol. effective amount of an anthranilamide compds. I (Markush included), an N-oxide thereof or an agriculturally suitable salt thereof, and (2) a film former or adhesive agent. Arthropodocidal composition containing anthranilamide compds. I may further comprise addnl. biol. active compds. selected from arthropodocides of the group consisting of pyrethroids, carbamates, neonicotinoids, neuronal sodium channel blockers, insecticidal macrocyclic lactones, γ -aminobutyric acid (GABA) antagonists, insecticidal ureas, and juvenile hormone mimics, and fungicides. The propagule is a seed of cotton, maize, soybean, rice, etc., or a rhizome, tuber, bulb or corm, or viable division thereof, of potato, sweet potato, garden onion, tulip, daffodil, crocus hyacinth, etc., or is a stem or leaf cutting.

IT 500007-98-7 500007-99-8 500008-13-9
 RL: AGR (Agricultural use); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)
 (anthranilamide compds. as pesticides for plant propagation material)

RN 500007-98-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[2-methyl-6-[[[1-(methyl-1-ethyl)amino]carbonyl]phenyl]-1-[2-[[[(trifluoroacetyl)amino]methyl]phenyl]-3-(trifluoromethyl)]- (9CI) (CA INDEX NAME)



RN 500007-99-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2-methyl-6-[[[1-(methyl-1-ethyl)amino]carbonyl]phenyl]-1-[2-[[[(trifluoroacetyl)amino]methyl]phenyl]-3-(trifluoromethyl)]- (9CI) (CA INDEX NAME)

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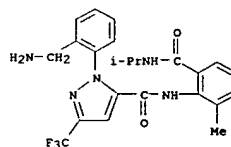
L9 ANSWER 17 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:242097 CAPLUS
 DOCUMENT NUMBER: 138:267201
 TITLE: Pesticidal compositions for coating plant propagation material containing anthranilamides
 INVENTOR(S): Berger, Richard Alan; Flexner, John Lindsey
 PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
 SOURCE: PCT Int. Appl., 147 pp.
 CODEN: PIXKDX
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003024222	A1	20030327	WO 2002-US30302	20020910
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SI, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2458163	A1	20030327	CA 2002-2458163	20020910
EP 1427285	A1	20040616	EP 2002-775972	20020910
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
BR 2002012993	A	20040817	BR 2002-12993	20020910
JP 2005502716	T	20050127	JP 2003-528126	20020910
JP 3770495	B2	20060426		
HU 200401893	A2	20050128	HU 2004-1893	20020910
NZ 532269	A	20051028	NZ 2002-532269	20020910
CN 1713819	A	20051228	CN 2002-818578	20020910
ZA 2004000413	A	20050120	ZA 2004-413	20040120
US 2004209923	A1	20041021	US 2004-485125	20040126
PRIORITY APPL. INFO.:			US 2001-323941P	P 20010921
			WO 2002-US30302	W 20020910

OTHER SOURCE(S): MARPAT 138:267201

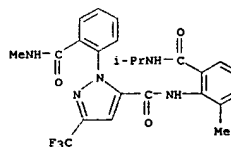
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L9 ANSWER 17 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 methyl-1-ethyl)amino]carbonyl]phenyl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 500008-13-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[(trifluoroacetyl)amino]methyl]phenyl]-1-[2-[[[(1-methyl-1-ethyl)amino]carbonyl]phenyl]-3-(trifluoromethyl)]- (9CI) (CA INDEX NAME)



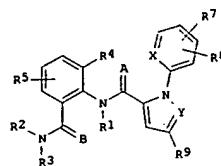
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 18 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:154408 CAPLUS
 DOCUMENT NUMBER: 138:205054
 TITLE: Preparation of substituted anthranilamides for controlling invertebrate pests
 INVENTOR(S): Finkelstein, Bruce Lawrence; Lahm, George Philip; McCann, Stephen Frederick; Song, Ying; Stevenson, Thomas Martin
 PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
 SOURCE: PCT Int. Appl., 105 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003016284	A1	20030227	WO 2002-US26960	20020813
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1417176	A1	20040512	EP 2002-761486	20020813
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
BR 2002012183	A	20040824	BR 2002-12183	20020813
JP 200503384	T	20050203	JP 2003-521210	20020813
CN 1653051	A	20050810	CN 2002-816050	20020813
US 2005282868	A1	20051222	US 2004-486312	20040722
PRIORITY APPLN. INFO.:			US 2001-312680P	P 20010816
			WO 2002-US26960	W 20020813

OTHER SOURCE(S): MARPAT 138:205054
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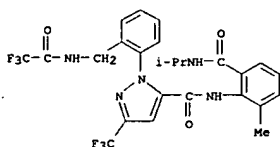
L9 ANSWER 18 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



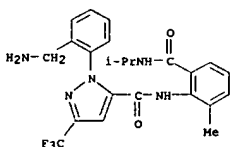
AB The title compds. [I; A, B = O, S; X = N, CR10; Y = N, CH; R1 = H, alkyl, cycloalkyl, etc.; R2 = alkyl, alkenyl, cycloalkyl, etc.; R3 = H, alkyl, alkenyl, etc.; NR2R3 = (un)substituted ring optionally containing addnl. heteroatom; R4 = alkyl, haloalkyl, CN, etc.; R5, R8 = H, alkyl, haloalkyl, etc.; R7 = H, alkyl, haloalkyl, etc.; R9 = CF3, OCF3, OCHF2, etc.; R10 = H, alkyl, haloalkyl, etc.], useful for controlling an invertebrate pest, were prepared E.g., a 3-step synthesis of I [A, B = O; X = CH; Y = N; R1 = H; R2 = iso-Pr; R3 = H; R4 = Me; R5 = H; R7 = 2-(CH2OH); R8 = H; R9 = CF3], starting from 1-[2-(methoxycarbonyl)phenyl]-3-trifluoromethyl-1H-pyrazole-5-carboxylic acid and 2-amino-3-methylbenzoic acid, which provided excellent levels of plant protection (20% or less damage) in biol. tests, was given.

IT 500007-98-7P 500028-35-3P
 RI: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) [preparation of substituted anthranilamides for controlling invertebrate pests]
 RN 500007-98-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[2-methyl-6-[[1-(1-methylethyl)amino]carbonyl]phenyl]-1-[2-[[1-(trifluoroacetyl)amino]methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 18 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 500028-35-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2-methyl-6-[[1-(1-methylethyl)amino]carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



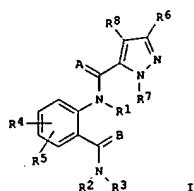
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L9 ANSWER 19 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:154 N4 CAPLUS
 DOCUMENT NUMBER: 138:200331
 TITLE: Method for controlling particular insect pests by applying anthranilamide compounds
 INVENTOR(S): Lahm, George Philip; McCann, Stephen Frederick; Patel, Kanu Maganbhai; Selby, Thomas Paul; Stevenson, Thomas Martin
 PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
 SOURCE: PCT Int. Appl., 150 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003015518	A1	20030227	WO 2002-US25613	20020813
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2454302	A1	20030227	CA 2002-2454302	20020813
EP 1416796	A1	20040512	EP 2002-752809	20020813
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
HU 200401043	A2	20040928	HU 2004-1043	20020813
BR 2002012187	A	20041005	BR 2002-12187	20020813
CN 1541063	A	20041027	CN 2002-815930	20020813
JP 2004538327	T	20041224	JP 2003-520289	20020813
JP 3689817	B2	20050831		
ZA 2004000033	A	20050803	ZA 2004-33	20020813
ZA 2004000034	A	20050803	ZA 2004-34	20020813
RU 2262231	C1	20051020	RU 2004-107513	20020813
NZ 530442	A	20060728	NZ 2002-530442	20020813
ZA 2003009911	A	20050311	ZA 2003-9911	20031222
US 2005075372	A1	20050407	US 2004-483115	20040107
JP 2005041880	A	20050217	JP 2004-258923	20040906
PRIORITY APPLN. INFO.:			US 2001-311919P	P 20010813
			US 2001-324173P	P 20010921
			US 2001-324128P	P 20010921
			US 2002-369661P	P 20020402
			JP 2003-520290	A3 20020813
			WO 2002-US25613	W 20020813

OTHER SOURCE(S): MARPAT 138:200331
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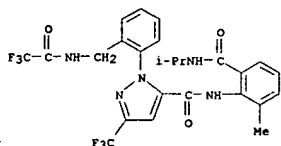
L9 ANSWER 19 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB Anthranilamide compds. I (Markush included), N-oxides or an agriculturally suitable salts thereof are prepared as insecticides for controlling lepidopteran, homopteran, hemipteran, thysanopteran and coleopteran insect pests. Insecticidal composition containing anthranilamide compds. I may further comprise addnl. biol. active compds. selected from arthropodocides of the group consisting of pyrethroids, carbamates, neonicotinoids, neuronal sodium channel blockers, insecticidal macrocyclic lactones, γ -aminobutyric acid (GABA) antagonists, insecticidal ureas, and juvenile hormone mimics.

IT 500007-98-7 500007-99-8 500008-13-9
 RL: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
 (anthranilamide compds. as insecticides)

RN 500007-98-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[2-methyl-6-[[[(1-methylethyl)amino]carbonyl]phenyl]-1-[2-[[[(trifluoroacetyl)amino]methyl]phenyl]-3-(trifluoromethyl)]]-9CI) (CA INDEX NAME)



RN 500007-99-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2-methyl-6-[[[(1-

L9 ANSWER 20 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:85815 CAPLUS
 DOCUMENT NUMBER: 138:395309
 TITLE: Development and validation of a liquid chromatography-mass spectrometric method for the determination of DPC 423, an antithrombotic agent, in rat and dog plasma

AUTHOR(S): Chi, Cecilia; Liang, Li; Padovani, Patty; Unger, Steve

CORPORATE SOURCE: Metabolism & Pharmacokinetics, PRI, Experimental Station, Bristol-Myers Squibb Company, Wilmington, DE, 19803-0353, USA

SOURCE: Journal of Chromatography, B: Analytical Technologies in the Biomedical and Life Sciences (2003), 783(1), 163-172
 CODEN: JCBAAI; ISSN: 1570-0232
 Elsevier Science B.V.

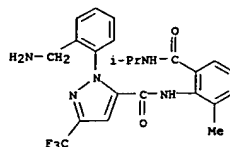
PUBLISHER: Journal
 DOCUMENT TYPE: English
 LANGUAGE: English

AB A sensitive and selective LC-MS-MS method for the determination of DPC 423 (I), an antithrombotic agent, is described. This method used a solid-phase extraction from 0.1 mL plasma with an Isolute C2 cartridge. HPLC separation was carried out on a YMC ODS-AQ C18 column (50x2 mm) at a flow rate of 300 μ L/min with an anal. time of 5 min. Compds. were eluted using a mobile phase of H₂O/CH₃CN/HCOOH:66:34:0.1 (volume/volume/volume), pH 4.0. A structural analog of I was used as the internal standard to account for variations in recovery and instrument response. Mass spectrometric detection was carried out with a PE Sciex API III+ triple quadrupole mass spectrometer equipped with a Turbo IonSpray source as the LC-MS interface. Good intraday and interday assay precision (<10% CV) and accuracy (<10% difference) were observed over a concentration range of 0.005-2.5 μ M in plasma. The extraction recoveries were approx. 90% and the method was found to be linear for the assay ($r^2 > 0.999$). The method has been successfully applied to discovery and preclin. pharmacokinetic studies, including a dose range-finding study and toxicokinetic exposure studies in rat and dog.

IT 292135-59-2, DPC 423
 RL: ANT (Analyte); PKT (Pharmacokinetics); ANST (Analytical study); BIOL (Biological study)
 (development and validation of liquid chromatog.-mass spectrometric method for determination of DPC 423 in rat and dog plasma)

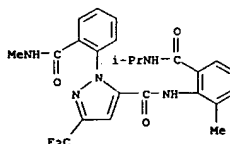
RN 292135-59-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 19 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 methylethyl)amino]carbonyl]phenyl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

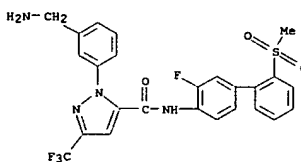
RN 500008-13-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[(methylamino)carbonyl]phenyl]-N-[2-methyl-6-[[[(1-methylethyl)amino]carbonyl]phenyl]-3-(trifluoromethyl)]]-9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L9 ANSWER 20 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



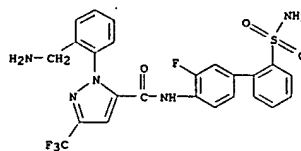
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REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L9 ANSWER 21 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:84721 CAPLUS
 DOCUMENT NUMBER: 139:255020
 TITLE: Inhibition of factor Xa reduces ischemic brain damage after thromboembolic stroke in rats
 AUTHOR(S): Wang, Xinkang; Xu, Lin; Wang, Hugh; Grzanna, Zhan, Yutian; Knabb, Robert M.; Luetgen, Joseph M.; Bozarth, Tracy A.; Galembo, Robert A.; Wong, Pancras C.; Bernard, Roberts; Vargas, Hugo; Chopp, Michael; Friedman, Steven M.; Feuerstein, Giora Z.
 CORPORATE SOURCE: Departments of Cardiovascular Sciences, Neurosciences,
 SOURCE: General Pharmacology, and Medicinal Chemistry, Bristol-Myers Squibb Company, Wilmington, DE, USA
 PUBLISHER: Stroke (2003), 34(2), 468-474
 CODEN: SJCCA7; ISSN: 0039-2499
 DOCUMENT TYPE: Lippincott Williams & Wilkins
 LANGUAGE: English
 AB Factor Xa (FXa) is a key coagulation protease and target for novel antithrombotic agents for prevention and treatment of diverse thromboembolic disorders. In the present study we describe the effect of a novel, potent, and selective FXa inhibitor, DPC602, on brain damage and neurobehavioral consequence in a rat thromboembolic model of stroke. Thromboembolic stroke was induced in rats by placement of an autologous clot into the middle cerebral artery. Laser-Doppler monitoring of cerebral blood flow demonstrated that DPC602 (8 mg/kg, single IV/IP bolus pretreatment) markedly improved cerebral blood flow after thromboembolic stroke by 25% to 160% (n = 6; P < 0.001) at 1 to 6 h. DPC602 demonstrated concentration- and time-dependent redns. in infarct size, with maximal effect (89% reduction; n = 14; P < 0.001) at the highest dose over controls. Neurol. function was also significantly improved in DPC602-treated rats at days 1, 3, and 7 (n = 13; P < 0.01). DPC602 treatment did not cause cerebral hemorrhage, assessed by free Hb in the ischemic brain tissues. These data suggest that anticoagulation with a selective FXa inhibitor might ameliorate the extent of ischemic brain damage and neurol. deficits after a thromboembolic event. Enhanced clot dissoln. and early reperfusion may account for the cerebrovascular-protective effect of the drug.
 IT 228258-45-5, DPC602
 RL: ADV (Adverse effect, including toxicity): PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (factor Xa inhibitor DPC602 in ischemic brain damage after thromboembolic stroke)
 RN 228258-45-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

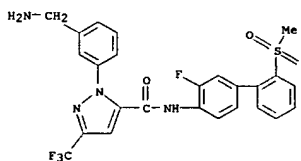
L9 ANSWER 21 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
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L9 ANSWER 22 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2002:932561 CAPLUS
 DOCUMENT NUMBER: 138:378909
 TITLE: Nonpeptide factor Xa inhibitors III: effects of DPC423, an orally-active pyrazole antithrombotic agent, on arterial thrombosis in rabbits
 AUTHOR(S): Wong, Pancras C.; Crain, Earl J.; Watson, Carol A.; Zaspel, Alverna M.; Wright, Matthew R.; Lam, Patrick T.; Pinto, Donald J. P.; Wexler, Ruth R.; Knabb, Robert M.
 CORPORATE SOURCE: Cardiovascular Biology, Bristol-Myers Squibb Company, Wilmington, DE, USA
 SOURCE: Journal of Pharmacology and Experimental Therapeutics (2002), 303(3), 993-1000
 CODEN: JPETAB; ISSN: 0022-3565
 PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB DPC423 [1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide] is a synthetic, competitive, and selective inhibitor of coagulation factor Xa (FXa) (Ki: 0.15 nM in humans, 0.3 nM in rabbit). The objective of this study was to compare effects of DPC423, enoxaparin (low-mol.-weight heparin), and argatroban (thrombin inhibitor) on arterial thrombosis and hemostasis in rabbit models of elec. induced carotid artery thrombosis and cuticle bleeding, resp. Compds. were infused i.v. continuously from 60 min before artery injury or cuticle transection to the end of experiment. Carotid blood flow was used as a marker of antithrombotic effect. Antithrombotic ED50 values were 0.4 mg/kg/h for enoxaparin (n = 6), 0.13 mg/kg/h for argatroban (n = 6), and 0.6 mg/kg/h for DPC423 (n = 12). DPC423 at the maximum antithrombotic dose increased activated partial thromboplastin time and prothrombin time (n = 6) by 1.8 ± 0.07- and 1.8 ± 0.13-fold, resp., without changes in thrombin time and ex vivo thrombin activity. The antithrombotic effect of DPC423 was significantly correlated with its ex vivo anti-FXa activity (r = 0.86). DPC423 at 1, 3, and 10 mg/kg p.o. increased carotid blood flow (percent control) at 45 min to 10 ± 4, 24 ± 6, and 74 ± 7, resp. (n = 6/group). Cuticle bleeding times (percent change over control) determined at the maximum antithrombotic dose were 88 ± 12 for argatroban, 69 ± 13 for heparin, 4 ± 3 for enoxaparin, 5 ± 4 for DPC423, and -3 ± 2 for the vehicle (n = 5-6/group), suggesting dissociation of antithrombotic and bleeding time effects for DPC423 and enoxaparin. The combination of aspirin and DPC423 at ineffective antithrombotic doses produced significant antithrombotic effect. Therefore, these results suggest that DPC423 is a clin. useful oral anticoagulant for the prevention of arterial thrombosis.
 IT 292135-59-2, DPC423
 RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (factor Xa inhibitors: orally-active pyrazole antithrombotic agent DPC423)
 RN 292135-59-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

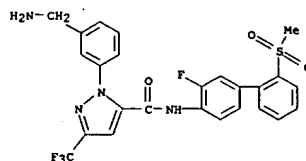
L9 ANSWER 22 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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 REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
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L9 ANSWER 23 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2002:845163 CAPLUS
 DOCUMENT NUMBER: 139:79
 TITLE: Nonpeptide factor Xa inhibitors: DPC423, a highly potent and orally bioavailable pyrazole
 antithrombotic
 agent
 AUTHOR(S): Wong, Pancras C.; Pinto, Donald J. P.; Knabb, Robert M.
 CORPORATE SOURCE: Cardiovascular Biology, Bristol-Myers Squibb Company, Wilmington, DE, USA
 SOURCE: Cardiovascular Drug Reviews (2002), 20(2), 137-152
 CODEN: CDREEA; ISSN: 0897-5957
 PUBLISHER: Neva Press
 DOCUMENT TYPE: Journal: General Review
 LANGUAGE: English
 AB A review. DPC 423 is a synthetic, orally bioavailable, competitive, and selective inhibitor of human coagulation factor Xa (Ki [nM]: factor Xa, 0.15; trypsin, 60; thrombin, 6000; plasma kallikrein, 61; activated protein C, 1800; factor IXa, 2200; factor VIIa, >15,000; chymotrypsin, >17,000; urokinase, >19,000; plasmin, >35,000; tissue plasminogen activator, >45,000; complement factor I, 44,000 [IC50]). In vitro, DPC 423 produced anticoagulant effects in human plasma in which it doubled prothrombin time, activated partial thromboplastin time, and Hestest clotting time at 3.1, 3.1, and 1.1 µM, resp. In dogs, DPC 423 had a good pharmacokinetic profile with an oral bioavailability of 57%, a plasma clearance of 0.24 L/kg/h, and a plasma half-life of 7.5 h. In rabbit and rat models of arteriovenous shunt thrombosis, DPC 423 was an effective antithrombotic agent with an IC50 of 150 and 470 nM, resp. The antithrombotic effect of DPC 423 is likely to be related to the inhibition of factor Xa but not to the inhibition of thrombin or due to direct inhibition of platelet aggregation. Therefore, based on potency, selectivity, efficacy, and oral bioavailability, DPC 423 was selected for clin. development as an oral anticoagulant for the potential treatment of thrombotic disorders. Preliminary human data suggest that DPC 423 is orally bioavailable in humans and has a long plasma half-life.
 IT 292135-59-2, DPC 423
 RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (DPC 423 as factor Xa inhibitor and highly potent and orally bioavailable antithrombotic agent)
 RN 292135-59-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

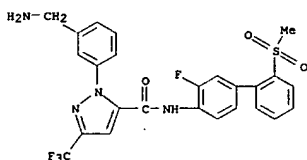
L9 ANSWER 23 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
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L9 ANSWER 24 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2002:621918 CAPLUS
 DOCUMENT NUMBER: 138:147036
 TITLE: DPC-423 (Bristol-Myers Squibb)
 AUTHOR(S): Tagliatella, Maurizio
 CORPORATE SOURCE: Section of Pharmacology, Department of Neuroscience, University of Naples "Federico II", Naples, 80131, Italy
 SOURCE: Current Opinion in Investigational Drugs (PharmaPress Ltd.) (2002), 3(2), 252-254
 CODEN: COIDA2; ISSN: 1472-4472
 PUBLISHER: PharmaPress Ltd.
 DOCUMENT TYPE: Journal: General Review
 LANGUAGE: English
 AB A review. DPC-423 is a biphenylamine-containing amide which is under development by Bristol-Myers Squibb (formerly DuPont Pharmaceuticals) as a Factor Xa inhibitor for the potential treatment of thrombotic disorders. As of August 2000, DPC-423 was in phase I trials. DPC-423 was discovered as a result of SAR modifications of DuPont's SN-429, including replacement of the benzamidine moiety with a less basic benzylamine. Its 2-aminomethylphenyl analog DPC-602 is also under investigation for thrombotic disorders.
 IT 292135-59-2, DPC-423
 RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (DPC-423 a factor Xa inhibitor).
 RN 292135-59-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

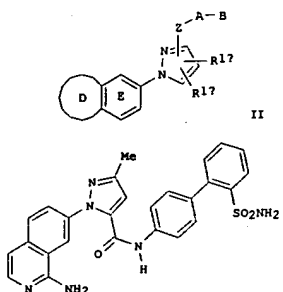
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
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L9 ANSWER 25 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2002:39605 CAPLUS
 DOCUMENT NUMBER: 136:102380
 TITLE: Preparation of novel guanidine mimics as factor Xa inhibitors
 INVENTOR(S): Lam, Patrick Y.; Clark, Charles G.; Dominguez, Celia; Fevig, John M.; Han, Qi; Li, Renhua; Pinto, Donald J. P.; Pruitt, James R.; Quan, Mimi L.
 SOURCE: Dupont Pharmaceuticals Company, USA
 U.S., 117 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6339099	B1	20020115	US 1998-99358	19980618
US 2002025963	A1	20020228	US 2001-924381	20010808
US 6906070	B2	20050614		
US 2003069258	A1	20030410	US 2002-98994	20020313
US 6958356	B2	20051025		
US 2004063772	A1	20040401	US 2003-602214	20030624
US 6963036	B2	20051115		
US 2006040973	A1	20060223	US 2005-197978	20050805
PRIORITY APPLN. INFO.:			US 1997-50265P	P 19970620
			US 1998-99358	A3 19980618
			US 2001-924381	B1 20010808
			US 2002-98994	A1 20020313

OTHER SOURCE(S): MARPAT 136:102380
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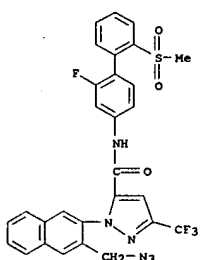
L9 ANSWER 25 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB The title compds. (I: ring D = 5-membered aromatic system containing from 1-2 heteroatoms selected from N, O, S; ring E is substituted with 0-2 R groups; ring E contains 0-2 N atom and is substituted by 0-1 R groups; R groups: Cl, F, Br, I, OH, alkoxy, amino(alkyl), (alkyl)amino; Z = bond, alkylene, (CH2)_rO(CH2)_r, (CH2)_rNR3(CH2)_r, (CH2)_rC(O)(CH2)_r, (CH2)_rC(O)O(CH2)_r, (CH2)_rOC(O)(CH2)_r, (CH2)_rC(O)NR3(CH2)_r, etc. provided that Z does not form a N-N, N-O, N-S, NCH2N, NCH2O, or NCH2S bond with ring M or group A; R1a-1b = H, alk(en)yl, aminoalkyl, alkoxy, alternatively, R1a-1b, when attached to adjacent carbon atoms, together with the atoms to which they are attached form a 5-8 membered (un)saturated ring (un)substituted and which contains from 0-2 heteroatoms selected from the group consisting of N, O, and S; alternatively, when Z is C(O)NH and R1a is attached to a ring carbon adjacent to Z, then R1a is a C(O) which replaces the amide hydrogen of Z to form a cyclic imide; R3 = H, alkyl, phenyl; A = (un)substituted carbocyclic, 5-10 membered heterocyclic system containing 1-4 heteroatoms selected from N, O, S; B = H, Y, X-Y; X = sulfonylalkyl, alkylsulfonyl, sulfonamide, etc.; Y = alkylamino, provided that X-Y does not form a N-N, O-N or S-N bond, carbocyclic group, 5-10 membered heterocyclic; r = 0-3; inhibitors of factor Xa which are useful in treating and preventing a thromboembolic disorder, were prepared and formulated. Thus, a multi-step synthesis of the title compound II, starting with 7-aminoisoquinoline, was described. A number of compds. I were found to exhibit a Ki of ≤ 15 μM against factor Xa.

IT 218299-04-8P

L9 ANSWER 25 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RECORD.

FORMAT

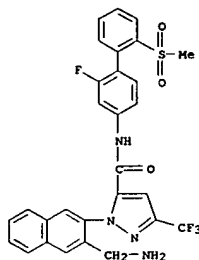
L9 ANSWER 25 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of novel guanidine mimics as factor Xa inhibitors)

RN 218299-04-8 CAPLUS

CN 1H-Pyrazole-5-carboxamide,

1-[3-(aminomethyl)-2-naphthalenyl]-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT 218302-16-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of novel guanidine mimics as factor Xa inhibitors)

RN 218302-16-0 CAPLUS

CN 1H-Pyrazole-5-carboxamide,

1-[3-(azidomethyl)-2-naphthalenyl]-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:88167 CAPLUS

DOCUMENT NUMBER: 136:160835

TITLE: Disposition of 1-[3-(Aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- 1H-pyrazole-5-carboxamide (DPC 423)

by Novel Metabolic Pathways. Characterization of Unusual Metabolites by Liquid Chromatography/Mass Spectrometry and NMR

AUTHOR(S): Mutlib, Abdul. E.; Shockcor, John; Chen, Shiang-Yuan; Espina, Robert J.; Pinto, Donald J.; Orwat, Michael J.; Prakash, Shimoga R.; Gan, Liang-Shang

CORPORATE SOURCE: Stine-Haskell Research Center, Drug Metabolism and Pharmacokinetics Section, DuPont Pharmaceuticals Company, Newark, DE, 19714, USA

SOURCE: Chemical Research in Toxicology (2002), 15(1), 48-62

CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

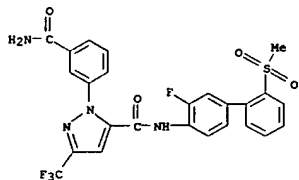
AB The in vitro and in vivo disposition of DPC 423 was investigated in mice, rats, dogs and humans and the metabolites characterized by LC/MS, LC/NMR and high field-NMR. The rodents produced several metabolites that included an aldehyde (M1), a carboxylic acid (M2), a benzyl alc. (M3), glutamate conjugates (M4 and M5), an acyl glucuronide (M6) and its isomers: a carbamyl glucuronide (M7); a phenol (M8) and its glucuronide conjugate (M9), two glutathione adducts (M10 and M11), a sulfamate conjugate (M12), isomers of an oxime metabolite (M13), and an amide (M14).

Humans and dogs produced less complex metabolite profiles than rats. While unchanged DPC 423 was the major component in plasma and urine samples, differences in the metabolic disposition of this compound among species were noted. M1 is believed to be rapidly oxidized to the carboxylic acid (M2), which forms the potentially reactive acyl glucuronide (M6). The formation of novel glutamate conjugates (M4 and M5) and their role in depleting endogenous glutathione have been described previously. The carbamyl glucuronide M7, found as the major metabolite

in rats and in other species, was considered nonreactive and was easily hydrolyzed to the parent compound in the presence of β-glucuronidase. The identification of GSH adducts M10 and M11 led us to postulate the existence of at least two reactive intermediates responsible for their formation, an epoxide and possibly a nitrile oxide, resp. Although the formation of GSH adducts such as M10 from epoxides has been described before, there are no reports to date describing the existence of a GSH adduct (M11) of an oxime. The formation of a sulfamate conjugate (M12) formed by direct coupling of sulfate to the nitrogen of benzylamine is described. A mechanism is proposed for the formation of the oxime (M13) that involves sequential oxidation of the benzylamine to the

corresponding hydroxylamine and nitroso intermediate. The rearrangement of the nitroso intermediate is believed to produce the oxime (M13). In vitro studies suggested that both the oxime (M13) and the aldehyde (M1) were precursors to the carboxylic acid (M2). This is the first demonstration of carboxylic acid formation via an oxime intermediate produced from an amine. The stability of DPC423 in plasma obtained from several species was studied. Significant species differences in the plasma stability of DPC 423 were observed. The formation of the aldehyde metabolite (M1) was

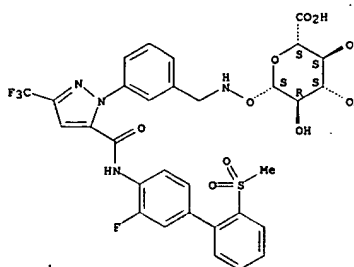
L9 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 found to be catalyzed by a semicarbazide-sensitive monoamine oxidase (SSAO) found in plasma of rabbits, dogs, and rhesus monkeys. Rat, chimpanzee, and human plasma did not form M1.
 IT 395095-29-1 395095-30-4 397249-90-0
 397249-91-1 397249-93-3 397249-94-4
 397249-95-5 397249-96-6 397249-97-7
 RL: ANT (Analyte); PKT (Pharmacokinetics); ANST (Analytical study); BIOL (Biological study)
 (disposition of DPC 423 by novel metabolic pathways and characterization of unusual metabolites by liquid chromatog./mass spectrometry and NMR)
 RN 395095-29-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-([3-(aminocarbonyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)(1,1'-biphenyl)-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 395095-30-4 CAPLUS
 CN β-D-Glucopyranuronic acid, 1-O-([3-[5-([3-fluoro-2'-(methylsulfonyl)(1,1'-biphenyl)-4-yl]amino)carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl)methyl]amino]- (9CI) (CA INDEX NAME)

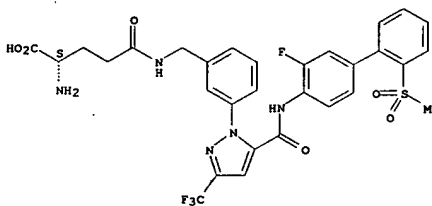
Absolute stereochemistry.

L9 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 397249-90-0 CAPLUS
 CN L-Glutamine, N-([3-[5-([3-fluoro-2'-(methylsulfonyl)(1,1'-biphenyl)-4-yl]amino)carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl)methyl]- (9CI) (CA INDEX NAME)

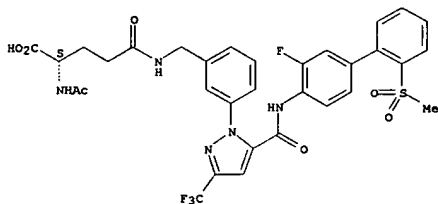
Absolute stereochemistry.



RN 397249-91-1 CAPLUS
 CN L-Glutamine, N2-acetyl-N-([3-[5-([3-fluoro-2'-(methylsulfonyl)(1,1'-biphenyl)-4-yl]amino)carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl)methyl]- (9CI) (CA INDEX NAME)

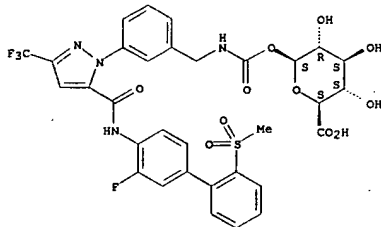
Absolute stereochemistry.

L9 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



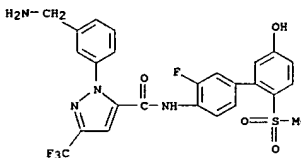
RN 397249-93-3 CAPLUS
 CN β-D-Glucopyranuronic acid, 1-([3-[5-([3-fluoro-2'-(methylsulfonyl)(1,1'-biphenyl)-4-yl]amino)carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl)methyl]carbamate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



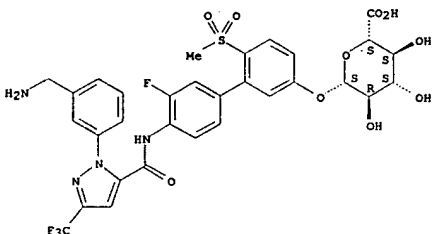
RN 397249-94-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-([3-(aminomethyl)phenyl]-N-[3-fluoro-5'-hydroxy-2'-(methylsulfonyl)(1,1'-biphenyl)-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 397249-95-5 CAPLUS
 CN β-D-Glucopyranosiduronic acid, 4'-([3-[5-([3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]-3'-fluoro-6-(methylsulfonyl)(1,1'-biphenyl)-3-yl (9CI) (CA INDEX NAME)

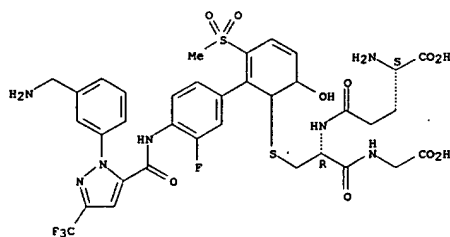
Absolute stereochemistry.



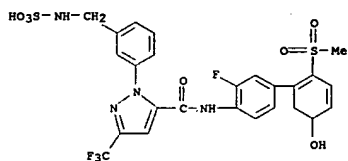
RN 397249-96-6 CAPLUS
 CN Glycine, L-γ-glutamyl-S-[2-[4-([3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]-3-fluorophenyl]-6-hydroxy-3-(methylsulfonyl)-2,4-cyclohexadien-1-yl]-L-cysteinyl- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 397249-97-7 CAPLUS
 CN Sulfamic acid, [(3-[5-[(2-fluoro-4-[5-hydroxy-2-(methylsulfonyl)-1,3-cyclohexadien-1-yl]phenyl]amino)carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl)methyl]- (9CI) (CA INDEX NAME)



IT 228258-45-5, DPC 602 292135-59-2, DPC 423
 RL: PKT (Pharmacokinetics); BIOL (Biological study)
 (disposition of DPC 423 by novel metabolic pathways and characterization of unusual metabolites by liquid chromatog./mass spectrometry and NMR)
 RN 228258-45-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro(1,1'-biphenyl)-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 27 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:881166 CAPLUS

DOCUMENT NUMBER: 136:144634

TITLE: P450-mediated metabolism of

1-[3-(aminomethyl)phenyl]-
 N-[3-fluoro-2'-(methylsulfonyl)-

3-(trifluoromethyl)-1H-pyrazole-5-carboxamide (DPC 423) and its analogs to aldoximes. Characterization

of glutathione conjugates of postulated intermediates derived from aldoximes

AUTHOR(S): Mutlib, Abdul E.; Chen, Shiang-Yuan; Espina, Robert J.; Shockcor, John; Prakash, Shimoga R.; Gan, Liang-Shang

CORPORATE SOURCE: Stine-Haskell Research Center, Drug Metabolism and Pharmacokinetics Section, DuPont Pharmaceuticals Company, Newark, DE, 19714, USA

SOURCE: Chemical Research in Toxicology (2002), 15(1), 63-75

CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

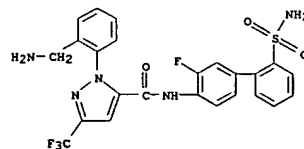
LANGUAGE: English

AB The in vivo and in vitro disposition of DPC 423, a highly potent, selective, and orally bioavailable inhibitor of blood coagulation factor Xa, has recently been described. Several metabolites, some of which were considered potentially reactive, were identified in rats. A novel GSH adduct, the structure of which was not determined conclusively, was isolated

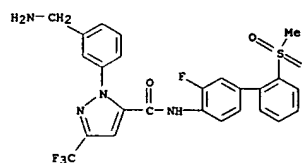
from bile of rats dosed with DPC 423. Herein, we describe the complete structural elucidation of this unique GSH conjugate employing LC/MS and high-field NMR. Similar GSH adducts of DPC 602, [13CD2]DPC 602, and SX 737, all structural analogs of DPC 423, were isolated, characterized spectroscopically, and shown to have identical mass fragmentation pathways. The structures of these conjugates were initially suspected to be either an amide with N-S bond or a nitrogen-oxygen juxtaposed amide with a C-S bond. Studies conducted with [13CD2]DPC 602 indicated an aldoxime structure. The concluding evidence came from HMBC NMR spectrum of the conjugate, which showed strong correlation of the cysteine methylene protons with the imino carbon. Further spectroscopic studies with chemical prepared GSH adduct from benzaldehyde oxime confirmed this pattern of correlation. In vivo and in vitro studies with the synthetic oxime intermediate from DPC 423 showed an adduct identical to the one isolated from the bile of rats dosed with DPC 423. This supported the intermediacy of an aldoxime as a precursor to the GSH adducts. It is postulated that the benzylamine moiety of DPC 423 (and its analogs) is oxidized to a hydroxylamine, which is subsequently converted to a nitroso intermediate. Subsequent rearrangement of the nitroso leads to an aldoxime which in turn is metabolized by P 450 to a reactive intermediate.

The formation of oxime from DPC 423 (and its analogs) was found to be mediated by rat CYP 3A1/2, which were also responsible for converting the oxime to the GSH trappable reactive intermediate. It is postulated that the aldoxime produces a radical or a nitrile oxide intermediate that reacts with GSH and hence produces this unusual GSH adduct. On the basis of synthetic analogy, it is more likely that the nitrile oxide resulting from two-electron oxidation of the aldoxime is the reactive intermediate. Intramolecular kinetic isotope effects were studied with [13CD2]DPC 602 to assess the importance of the metabolic cleavage of the aminomethyl carbon-hydrogen bond in forming this GSH adduct. The lack of isotope

L9 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 292135-59-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)(1,1'-biphenyl)-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS

FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

L9 ANSWER 27 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

effect in forming the aldoxime from [13CD2]DPC 602 suggests its formation does not occur through the imine intermediate. Instead the data supports the postulated mechanism of hydroxylamine and nitroso intermediates as precursors to the aldoxime. However, the formation of the GSH adduct

from [13CD2]DPC 602 did show a significant intramolecular kinetic isotope effect (KH/KD = 2.3) since a carbon-deuterium bond had to be broken on the aldoxime prior to the formation of the adduct. A stable nitrile oxide derived from DPC 602 was postulated as the reactive intermediate responsible for forming this unique GSH adduct.

IT 228258-45-5P, DPC 602 228258-46-6P, SX 737

292135-59-2P, DPC 423 395095-27-9P 395095-29-1P

395095-30-4P 395095-32-6P 395685-16-2P,

[13CD2]DPC 602

RL: PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic

preparation); BIOL (Biological study); PREP (Preparation)

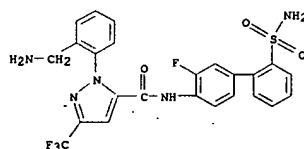
(P 450-mediated metabolism of blood coagulation factor Xa inhibitor

DPC 423 and its analogs to aldoximes: characterization of glutathione conjugates)

RN 228258-45-5 CAPLUS

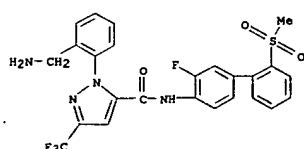
CN 1H-Pyrazole-5-carboxamide,

1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro(1,1'-biphenyl)-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 228258-46-6 CAPLUS

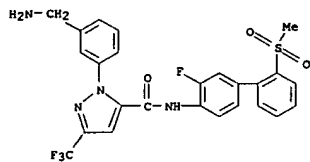
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)(1,1'-biphenyl)-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 292135-59-2 CAPLUS

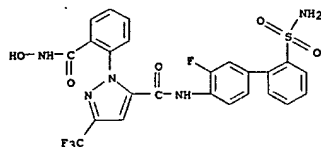
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-

L9 ANSWER 27 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



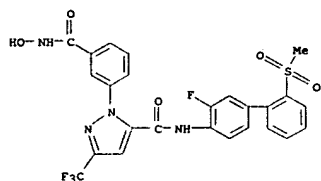
• HCl

RN 395095-27-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-1-[2-[(hydroxyamino)carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

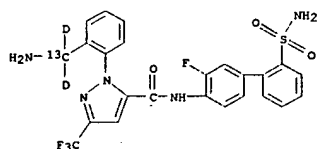


RN 395095-29-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 27 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

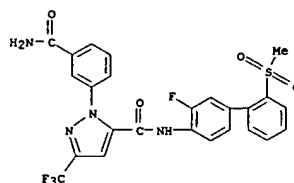


RN 395685-16-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl-13C-d2)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



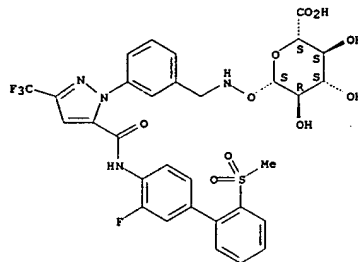
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L9 ANSWER 27 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 395095-30-4 CAPLUS
CN β-D-Glucopyranuronic acid, 1-O-[[[3-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



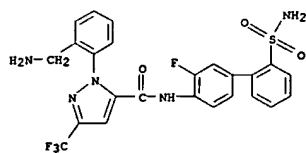
RN 395095-32-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[3-[(hydroxyamino)carbonyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 28 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN

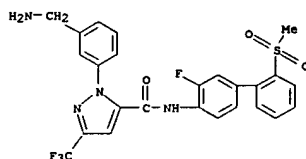
ACCESSION NUMBER: 2001:705983 CAPLUS
DOCUMENT NUMBER: 136:79226
TITLE: Formation of unusual glutamate conjugates of 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide (DPC 423) and its analogs: the role of γ-glutamyltranspeptidase in the biotransformation of benzylamines
AUTHOR(S): Mutlib, Abdul; Shockcor, John; Chen, Shiang-Yuan; Espina, Robert; Lin, Jianrong; Graciani, Nilsa; Prakash, Shimoga; Gan, Liang-Shang
CORPORATE SOURCE: Drug Metabolism and Pharmacokinetics Section, Stine-Haskell Research Center, DuPont Pharmaceuticals Company, Newark, DE, 19714, USA
SOURCE: Drug Metabolism and Disposition (2001), 29(10), 1296-1306
CODEN: DMDSAI; ISSN: 0090-9556
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The role of γ-glutamyltranspeptidase (GGT) in transferring glutamate from endogenous glutathione (GSH) to the benzylamine moiety of a compound, such as 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide (DPC 423), is described. Studies were performed with structurally related analogs of DPC 423 to demonstrate that this type of reaction was common to compounds possessing a benzylamine group. Synthesizing appropriate standards and confirming by liquid chromatography (LC)/mass spectroscopy and LC/NMR made unambiguous assignments of the structures of glutamate conjugates of DPC 423. The use of stable isotope-labeled GSH for metabolism studies has not been described before. In the present study, we report the novel use of deuterated GSH in conjunction with mass spectral analysis to demonstrate the glutamate transfer to the benzylamines in the presence of GGT. To further demonstrate that the α protons on the benzylamines and glutamate (as part of glutathione) were unaffected during the transpeptidation, these protons were replaced with deuterium. Acivicin (AT-125), a potent and selective inhibitor of GGT, was used to abolish the formation of the glutamate conjugates of DPC 423 in vitro and in vivo. This provided further evidence of the role of GGT in forming the glutamate conjugates of benzylamines. This study demonstrated conclusively that GGT was responsible for mediating the transfer of glutamic acid from GSH to the benzylamine moiety of a series of structurally related compounds.
IT 228258-45-5 292135-59-2, DPC 423 292135-59-2D, DPC 423, glutamate conjugates
RL: PKT (Pharmacokinetics); BIOL (Biological study) (formation of unusual glutamate conjugates of DPC 423 and its analogs and role of γ-glutamyltranspeptidase in the biotransformation of benzylamines)
RN 228258-45-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10519356a.trn

L9 ANSWER 28 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



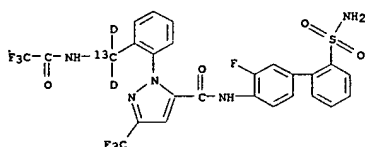
RN 292135-59-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

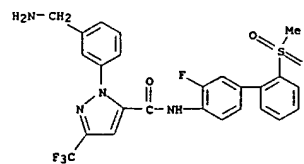
RN 292135-59-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-13C-d2]phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 28 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 yll-1-[2-[(trifluoroacetyl)amino]methyl-13C-d2]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



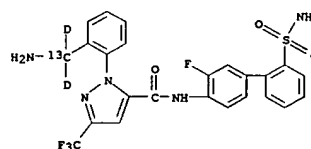
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L9 ANSWER 28 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

IT 385380-71-2P
 RL: PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (formation of unusual glutamate conjugates of DPC 423 and its analogs and role of γ -glutamyltranspeptidase in the biotransformation of benzylamines)
 RN 385380-71-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-13C-d2]phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



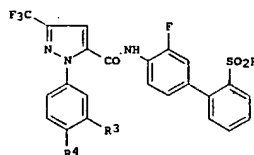
● HCl

IT 385380-68-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (formation of unusual glutamate conjugates of DPC 423 and its analogs and role of γ -glutamyltranspeptidase in the biotransformation of benzylamines)
 RN 385380-68-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-

L9 ANSWER 29 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:300687 CAPLUS
 DOCUMENT NUMBER: 134:311206
 TITLE: Preparation of 1,3,5-trisubstituted pyrazoles for pharmaceutical use as factor Xa inhibitors
 INVENTOR(S): Zhou, Jiacheng; Oh, Lynette May; Confalone, Pasquale N.; Li, Hui-yin; Ma, Philip
 PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
 SOURCE: PCT Int. Appl., 103 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001029006	A1	20010426	WO 2000-US29031	20001020
W: AU, BR, CA, CH, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, K2, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6329527	B1	20011211	US 2000-685127	20001010
CA 2382212	A1	20010426	CA 2000-2382212	20001020
EP 1222172	A1	20020717	EP 2000-972292	20001020
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY				
US 2002055641	A1	20020509	US 2001-5938	20011203
US 6465656	B2	20021015		
PRIORITY APPLN. INFO.:			US 1999-161666P	P 19991021
			US 2000-685127	A3 20001010
			WO 2000-US29031	W 20001020

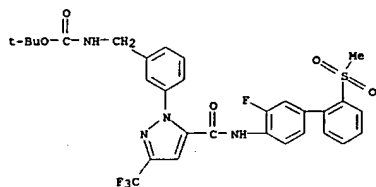
OTHER SOURCE(S): MARPAT 134:311206
 GI



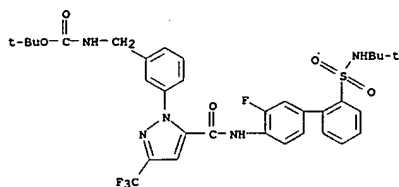
AB 1,3,5-Trisubstituted pyrazoles, such as I [R = Me, NH2; R3 = CN, CH2NH2; R4 = H, F], were prepared for pharmaceutical use as factor Xa inhibitors (no biol. testing data presented). Thus, I (R = Me, R3 = CN, R4 = H) was

L9 ANSWER 29 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 IT prepd. via cyclization of F3CONHNHCH4-3-CN with H2C:CHCONHCH3(-2-F)-4-C6H4-2-SO2Me and subsequent dehydrogenation of the resulting pyrazoline using N-chlorosuccinimide.
 335275-82-6P 335275-91-7P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (preparation of 1,3,5-trisubstituted pyrazoles for pharmaceutical use)

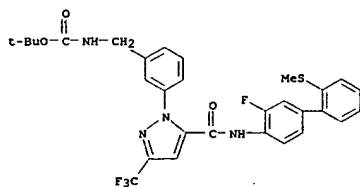
as factor Xa inhibitors)
 RN 335275-91-7 CAPLUS
 CN Carbamic acid, [[3-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



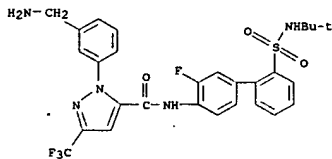
RN 335275-91-7 CAPLUS
 CN Carbamic acid, [[3-[5-[[[2'-[[[1,1-dimethylethyl]amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 29 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CN Carbamic acid, [[3-[5-[[[3-fluoro-2'-(methylthio)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 335275-92-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-[[[1,1-dimethylethyl]amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



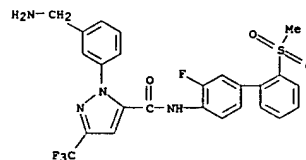
● HCl

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RECORD.

FORMAT

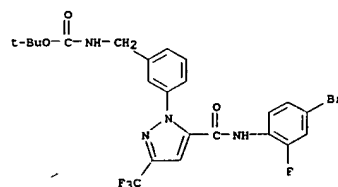
L9 ANSWER 29 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 IT 292135-59-2P 335275-89-3P 335275-90-6P
 335275-92-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of 1,3,5-trisubstituted pyrazoles for pharmaceutical use)

as factor Xa inhibitors)
 RN 292135-59-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 335275-89-3 CAPLUS
 CN Carbamic acid, [[3-[5-[[[4-bromo-2-fluorophenyl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 335275-90-6 CAPLUS

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:55833 CAPLUS
 DOCUMENT NUMBER: 134:246871
 TITLE: Discovery of 1-[3-(Aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide (DPC423), a Highly Potent, Selective, and Orally Bioavailable Inhibitor of Blood Coagulation Factor Xa
 AUTHOR(S): Pinto, Donald J. P.; Orwat, Michael J.; Wang, Shuaige; Fevig, John M.; Quan, Mimi L.; Amparo, Eugene; Cacciola, Joseph; Rossi, Karen A.; Alexander, Richard S.; Smallwood, Angela M.; Luetttgen, Joseph M.; Liang, Li; Aungst, Bruce J.; Wright, Matthew R.; Knabb, Robert M.; Wong, Pancras C.; Wexler, Ruth R.; Lam, Patrick Y. S.
 CORPORATE SOURCE: DuPont Pharmaceuticals Company, Wilmington, DE, 19880-0500, USA
 SOURCE: Journal of Medicinal Chemistry (2001), 44(4), 566-578
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:246871
 AB Factor Xa (fXa) plays a critical role in the coagulation cascade, serving as the point of convergence of the intrinsic and extrinsic pathways. Together with nonenzymic cofactor Va and Ca2+ on the phospholipid surface of platelets or endothelial cells, factor Xa forms the prothrombinase complex, which is responsible for the proteolysis of prothrombin to catalytically active thrombin. Thrombin, in turn, catalyzes the cleavage of fibrinogen to fibrin, thus initiating a process that ultimately leads to clot formation. Recently, the authors reported on a series of isoxazoline and isoxazole monobasic noncovalent inhibitors of factor Xa which show good potency in animal models of thrombosis. In this paper, the authors wish to report on the optimization of the heterocyclic core, which ultimately led to the discovery of a novel pyrazole SN429 (fXa Ki = 13 pM). The authors also report on the authors efforts to improve the oral bioavailability and pharmacokinetic profile of this series while maintaining subnanomolar potency and in vitro selectivity. This was achieved by replacing the highly basic benzamidine P1 with a less basic benzylamine moiety. Further optimization of the pyrazole core substitution and the biphenyl P4 culminated in the discovery of DPC423, a highly potent, selective, and orally active factor Xa inhibitor which was chosen for clin. development.

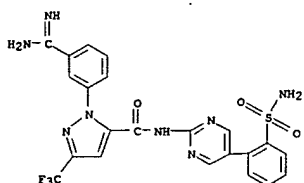
IT 209955-39-5P 209955-61-3P 209957-34-6P
 209957-36-8P 209957-48-2P 209957-52-8P
 292135-59-2P, DPC 423
 RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
 (discovery of pyrazolecarboxamide derivative (DPC423) as a highly potent and orally bioavailable inhibitor of blood coagulation factor Xa with good pharmacokinetics and structure-activity relationships)

RN 209955-39-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 (aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-38-4
 CMF C22 H17 F3 N8 O3 S



CM 2

CRN 76-05-1
 CMF C2 H F3 O2



RN 209955-61-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-60-2
 CMF C24 H20 F3 N5 O3 S

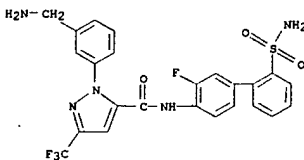
L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CRN 76-05-1
 CMF C2 H F3 O2



RN 209957-36-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-
 3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-35-7
 CMF C24 H19 F4 N5 O3 S



CM 2

CRN 76-05-1
 CMF C2 H F3 O2



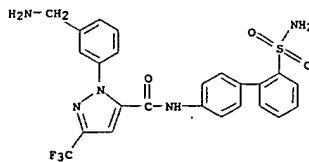
RN 209957-48-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-47-1

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L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

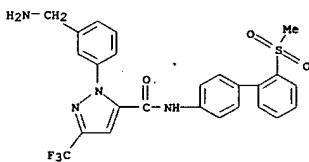
CRN 76-05-1
 CMF C2 H F3 O2



RN 209957-34-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

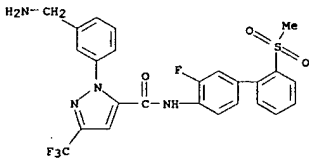
CM 1

CRN 209957-33-5
 CMF C25 H21 F3 N4 O3 S



CM 2

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CMF C25 H20 F4 N4 O3 S



CM 2

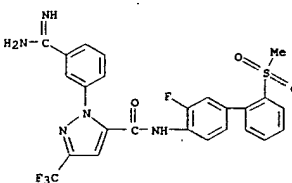
CRN 76-05-1
 CMF C2 H F3 O2



RN 209957-52-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-51-7
 CMF C25 H19 F4 N5 O3 S

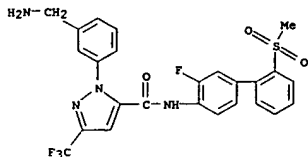


CM 2

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CRN 76-05-1
CMF C2 H F3 O2



RN 292135-59-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



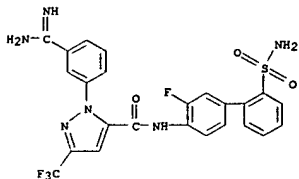
● HCl

IT 209954-60-9P 209955-28-2P 209957-54-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (discovery of pyrazolecarboxamide derivative (DPC423) as a highly potent and orally bioavailable inhibitor of blood coagulation factor Xa with good pharmacokinetics and structure-activity relationships)
RN 209954-60-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)
CM 1
CRN 209954-59-6
CMF C24 H19 F3 N6 O3 S

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CM 2
CRN 76-05-1
CMF C2 H F3 O2



RN 209957-54-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)
CM 1
CRN 209957-53-9
CMF C24 H18 F4 N6 O3 S

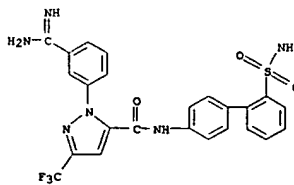


CM 2
CRN 76-05-1
CMF C2 H F3 O2



RN 331006-14-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

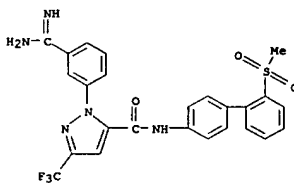


CM 2
CRN 76-05-1
CMF C2 H F3 O2

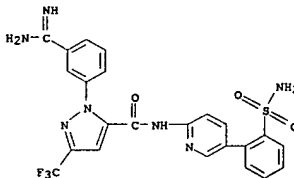


RN 209955-28-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1
CRN 209954-94-9
CMF C25 H20 F3 N5 O3 S



L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CM 1
CRN 209955-48-6
CMF C23 H18 F3 N7 O3 S

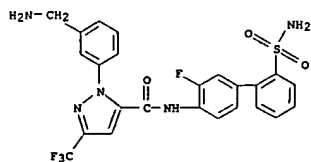


CM 2
CRN 76-05-1
CMF C2 H F3 O2



IT 209957-35-7
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (discovery of pyrazolecarboxamide derivative (DPC423) as a highly potent and orally bioavailable inhibitor of blood coagulation factor Xa with good pharmacokinetics and structure-activity relationships)
RN 209957-35-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

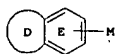


REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L9 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2000:725629 CAPLUS
 DOCUMENT NUMBER: 133:296430
 TITLE: Preparation of aryl sulfonyls as factor Xa inhibitors
 INVENTOR(S): Wexler, Ruth R.; Jacobson, Irina C.
 PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
 SOURCE: PCT Int. Appl., 116 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

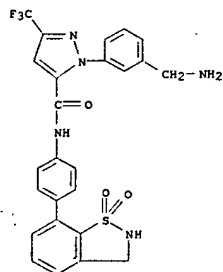
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000059902	A2	20001012	WO 2000-US8364	20000330
WO 2000059902	A3	20010426		
W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2368630	A1	20001012	CA 2000-2368630	20000330
EP 1175419	A2	20020130	EP 2000-923096	20000330
EP 1175419	B1	20030528		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 241621	T	20030615	AT 2000-923096	20000330
ES 2197092	T3	20040101	ES 2000-923096	20000330
US 6399644	B1	20020604	US 2000-540467	20000331
US 2003050315	A1	20030313	US 2002-74301	20020212
US 6689770	B2	20040210		
PRIORITY APPLN. INFO.:				
			US 1999-127634P	P 19990402
			WO 2000-US8364	W 20000330
			US 2000-540467	A3 20000331

OTHER SOURCE(S): MARPAT 133:296430
 GI



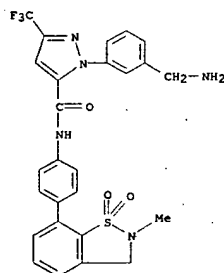
AB Aryl sulfonyls I [ring D is absent or is CH2N:CH, CH:NCH2, aromatic system containing heteroatoms, etc.; E = Ph, pyridyl, pyrazinyl, etc.; M = heterocyclyl], effective factor Xa inhibitors (no data), were prepared E.g., N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-1-(4-

L9 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 IT methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide was prepd.
 300710-16-1P 300710-17-2P 300710-18-3P
 300710-21-8P 300710-22-9P 300710-23-0P
 300710-24-1P 300710-28-5P 300710-33-2P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of aryl sulfonyls as factor Xa inhibitors)
 CN 300710-16-1 CAPLUS
 RN 1H-Pyrazole-5-carboxamide,
 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

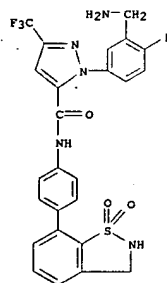


RN 300710-17-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

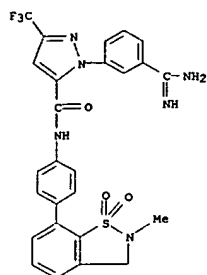


RN 300710-18-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



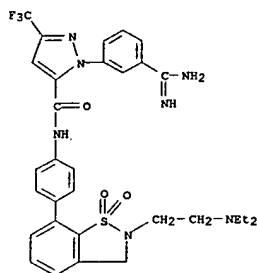
RN 300710-21-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 300710-22-9 CAPLUS

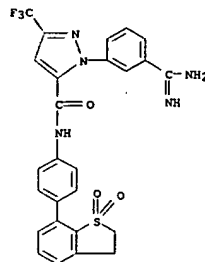
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-{2-[(diethylamino)ethyl]-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl}phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 300710-23-0 CAPLUS

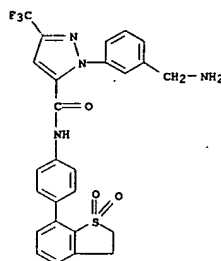
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-{2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl}phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 300710-24-1 CAPLUS

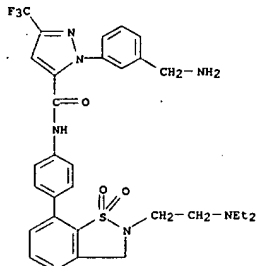
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-{2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl}phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 300710-28-5 CAPLUS

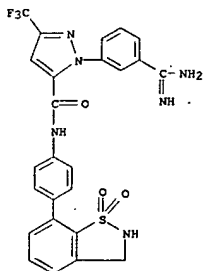
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-{2-[(diethylamino)ethyl]-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl}phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 300710-33-2 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-{2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl}phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT 300710-45-6P

RI: ACT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

RN 300710-45-6 CAPLUS

CN 1,2-Benzisothiazole-2(3H)-carboxylic acid, 7-[4-{[1-[3-(aminomethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl}amino]phenyl]-, 1,1-dimethylethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)

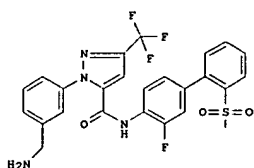
10519356a.trn

L9 ANSWER 32 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 AB Provided is a method of treating thrombosis in mammals by administering therapeutically effective amts. of a combination of (i) a Factor Xa inhibitor, and (ii) a compound selected from the group consisting of aspirin, TPA, a GPIIb/IIIa antagonist, low mol. weight heparin and heparin, wherein the dose administered for at least one of (i) and (ii) is a subtherapeutic dose. Preferably, the combination of (i) and (ii) provides a synergistic effect. A combination of I (Factor Xa inhibitor) and aspirin at their subtherapeutic doses produced a significant antithrombotic effect in a rabbit model of arterial thrombosis. Pharmaceutical dosage forms are discussed.

INVENTOR(S): Wong, Pancras C.
 PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
 SOURCE: PCT Int. Appl., 38 pp.
 CODEN: PIXXDZ
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000053264	A1	20000914	WO 2000-US6451	20000310
W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6794412	B1	20040921	US 2000-519188	20000306
CA 2361650	A1	20000914	CA 2000-2361650	20000310
EP 1161279	A1	20011212	EP 2000-913894	20000310
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000010381	A	20020205	BR 2000-10381	20000310
AU 766089	B2	20031009	AU 2000-35254	20000310
NZ 513217	A	20031128	NZ 2000-513217	20000310
ZA 2001006360	A	20020802	ZA 2001-6360	20010802
PRIORITY APPLN. INFO.:			US 1999-123815P	P 19990311
			WO 2000-US6451	W 20000310

GI



I

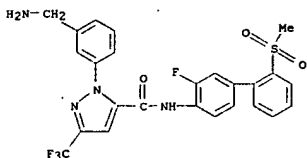
L9 ANSWER 32 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209957-48-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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CRN 209957-47-1
 CMF C25 H20 F4 N4 O3 S



CM 2

CRN 76-05-1
 CMF C2 H F3 O2

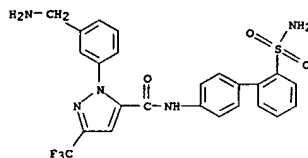


RN 292135-59-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 32 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 AB Provided is a method of treating thrombosis in mammals by administering therapeutically effective amts. of a combination of (i) a Factor Xa inhibitor, and (ii) a compound selected from the group consisting of aspirin, TPA, a GPIIb/IIIa antagonist, low mol. weight heparin and heparin, wherein the dose administered for at least one of (i) and (ii) is a subtherapeutic dose. Preferably, the combination of (i) and (ii) provides a synergistic effect. A combination of I (Factor Xa inhibitor) and aspirin at their subtherapeutic doses produced a significant antithrombotic effect in a rabbit model of arterial thrombosis. Pharmaceutical dosage forms are discussed.

IT 209955-61-3 209957-48-2 292135-59-2
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (antithrombotic combination of a Factor Xa inhibitor and aspirin, TPA, a GPIIb/IIIa antagonist, or heparin derivative)
 RN 209955-61-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

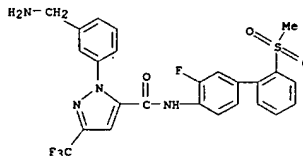
CM 1
 CRN 209955-60-2
 CMF C24 H20 F3 N5 O3 S



CM 2

CRN 76-05-1
 CMF C2 H F3 O2

L9 ANSWER 32 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



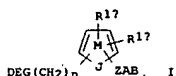
● HCl

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2000:83115 CAPLUS
 DOCUMENT NUMBER: 132:137392
 TITLE: Preparation of azoles as Factor Xa inhibitors.
 INVENTOR(S): Pinto, Donald Joseph Phillip; Pruitt, James Russell;
 Cacciola, Joseph; Fevig, John Matthew; Han, Qi;
 ORwat,
 Michael James; Quan, Mimi Lifan; Rossi, Karen Anita
 PATENT ASSIGNEE(S): Dupont Pharmaceuticals Co., USA
 SOURCE: U.S., 152 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6020357	A	20000201	US 1997-995834	19971222
US 6548512	B1	20030415	US 2000-492708	20000127
PRIORITY APPLN. INFO.:			US 1996-33437P	P 19961223
			US 1997-50304P	P 19970620
			US 1997-995834	A3 19971222

OTHER SOURCE(S): MARPAT 132:137392
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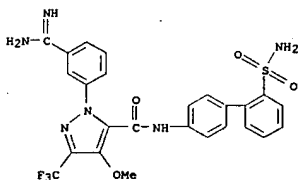


AB Title compds. [I: ring M contains, in addition to J, 0-3 N atoms; J = N,
 NH;
 D = CN, C((NR8)NR7R9, C(O)NR7R8, etc.; E = (un)substituted Ph, pyridyl,
 pyrimidinyl, etc.; DEG = R-substituted pyridyl; R = H, halo, CF3, etc.; G
 = absent, NHCH2, OCH2, etc.; Z = Cl-4 alkylene, (CH2)RO(CH2)R, etc.; R1a,
 R1b = absent, NMe, OMe, etc.; A = (un)substituted C3-10 carbocyclic
 residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms
 selected
 from N, O, and S; B = (un)substituted C3-10 carbocyclic residue, 5-10
 membered heterocyclic containing from 1-4 heteroatoms selected from N,
 O, and
 S, etc.; R7 = H, OH, Cl-6 alkyl, etc.; R8, R9 = H, Cl-6 alkyl, (CH2)nPh;
 n
 = 0-3; r = 0-3; s = 0-2; with provisos], useful as inhibitors of factor
 Xa, were prepared and formulated. Thus, treatment of 4-[o-(tert-
 BuSO2)phenyl]aniline with Me3Al/hexane in CH2Cl2 followed by the
 addition of
 Me 1-(3-cyanophenyl)imidazol-2-ylcarboxylate (preparation described),
 and the

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 RN 209954-62-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-
 (aminosulfonyl)[1,1'-biphenyl]-4-yl]-4-methoxy-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-61-0
 CMF C25 H21 F3 N6 O4 S



CM 2

CRN 76-05-1
 CMF C2 H F3 O2



RN 209954-94-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-
 (methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
 INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 Plimmer reaction of the resulting intermediate afforded
 1-[3-(aminoiminomethyl)-2-[(2'-aminosulfonyl)-1,1'-biphen-4-
 yl]amino]carbonyl]imidazole. Several I showed Ki ≤10 μM against
 Factor Xa and thrombin.

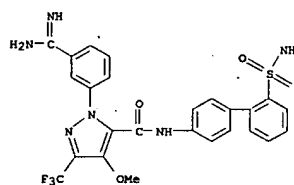
IT 209954-61-0P 209954-62-1P 209954-94-9P
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 209955-27-1P 209955-28-2P 209955-37-3P
 209955-41-9P 209955-44-2P 209955-45-3P
 209955-46-4P 209955-47-5P 209955-48-6P
 209955-49-7P 209955-50-0P 209955-51-1P
 209955-52-2P 209955-53-3P 209955-60-2P
 209955-61-3P 209956-54-7P 209956-70-7P
 209956-75-2P 209956-76-3P 209956-77-4P
 209956-78-5P 209956-99-0P 209957-00-6P
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 209957-33-5P 209957-34-6P 209957-35-7P
 209957-36-8P 209957-38-0P 209957-40-4P
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 209958-33-8P 256512-05-7P 256512-19-3P
 256512-30-8P

RL: BAC (Biological activity or effector, except adverse); BSU

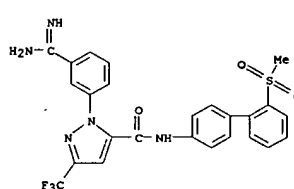
(Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of azoles as Factor Xa inhibitors)

RN 209954-61-0 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-
 (aminosulfonyl)[1,1'-biphenyl]-4-yl]-4-methoxy-3-(trifluoromethyl)- (9CI)
 (CA INDEX NAME)

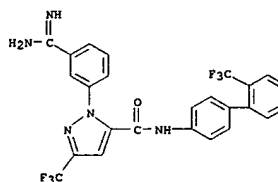


L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



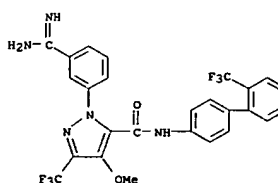
RN 209954-95-0 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-
 (trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]- (9CI)
 (CA INDEX NAME)



RN 209954-96-1 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-
 (trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]- (9CI)
 (CA INDEX NAME)

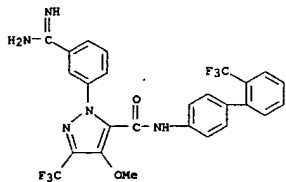


L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209955-26-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-4-methoxy-3-(trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-96-1
 CMF C26 H19 F6 N5 O2



CM 2

CRN 76-05-1
 CMF C2 H F3 O2



RN 209955-27-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-3-(trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-95-0
 CMF C25 H17 F6 N5 O

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 2

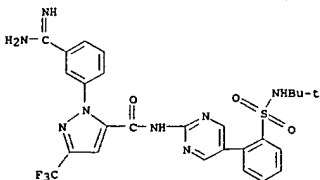
CRN 76-05-1
 CMF C2 H F3 O2



RN 209955-37-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-[(1,1-dimethylethyl)amino]sulfonyl]phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-36-2
 CMF C26 H25 F3 N8 O3 S



CM 2

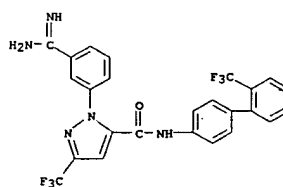
CRN 76-05-1
 CMF C2 H F3 O2



RN 209955-41-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, trifluoroacetate (2:1) (9CI) (CA INDEX NAME)

10519356a.trn

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

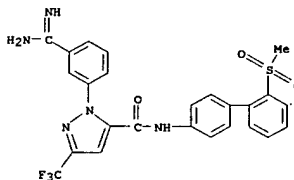
CRN 76-05-1
 CMF C2 H F3 O2



RN 209955-28-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

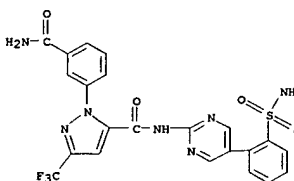
CRN 209954-94-9
 CMF C25 H20 F3 N5 O3 S



L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 209955-40-8
 CMF C22 H16 F3 N7 O4 S

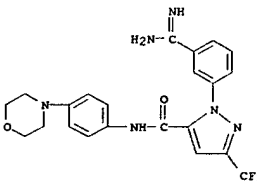


CM 2

CRN 76-05-1
 CMF C2 H F3 O2



RN 209955-44-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

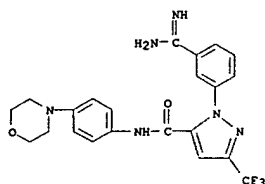


RN 209955-45-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)-, tris(trifluoroacetate) (9CI)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(CA INDEX NAME)

CM 1

CRN 209955-44-2
CMF C22 H21 F3 N6 O2



CM 2

CRN 76-05-1
CMF C2 H F3 O2

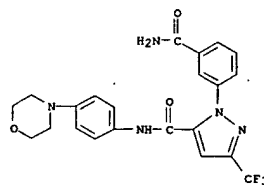


RN 209955-46-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 209955-46-4
CMF C22 H20 F3 N5 O3

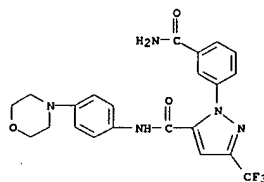


RN 209955-47-5 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-46-4
CMF C22 H20 F3 N5 O3



CM 2

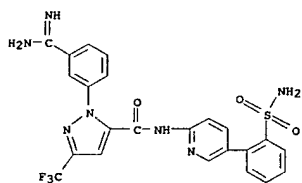
CRN 76-05-1
CMF C2 H F3 O2



L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209955-48-6 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

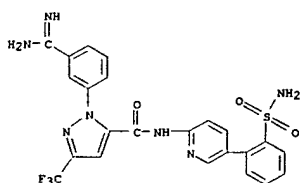


RN 209955-49-7 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-48-6
CMF C23 H18 F3 N7 O3 S



CM 2

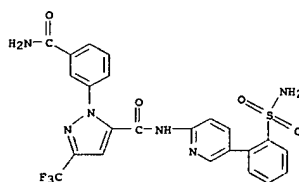
CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 209955-50-0
CMF C23 H17 F3 N6 O4 S

RN 209955-50-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

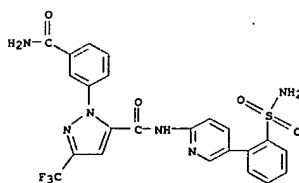


RN 209955-51-1 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-50-0
CMF C23 H17 F3 N6 O4 S



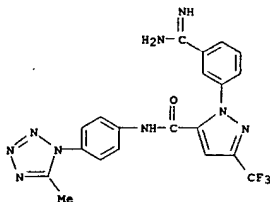
CM 2

CRN 76-05-1

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C2 H F3 O2



RN 209955-52-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5-methyl-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209955-53-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5-methyl-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

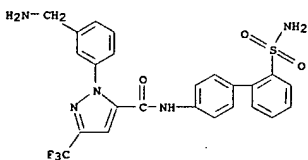
CM 1

CRN 209955-52-2
CMF C20 H16 F3 N9 O

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 209955-60-2
CMF C24 H20 F3 N5 O3 S

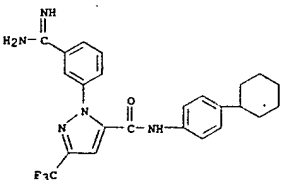


CM 2

CRN 76-05-1
CMF C2 H F3 O2

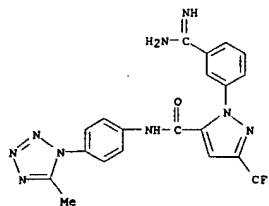


RN 209956-54-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(cyclohexylphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209956-70-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-chloro-4-(morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

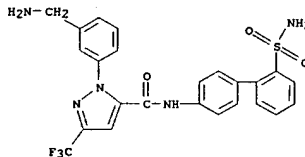


CM 2

CRN 76-05-1
CMF C2 H F3 O2

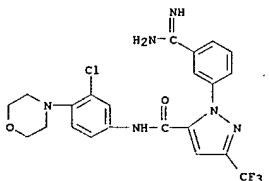


RN 209955-60-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

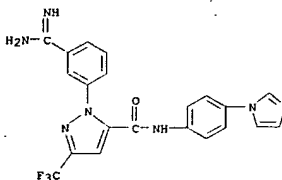


RN 209955-61-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209956-75-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

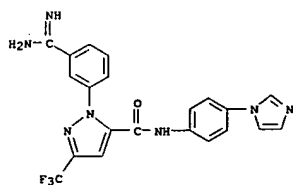


RN 209956-76-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209956-75-2
CMF C21 H16 F3 N7 O

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

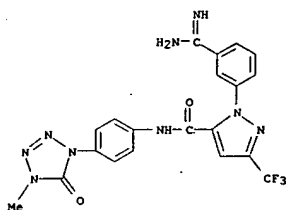
CRN 76-05-1

CMF C2 H F3 O2



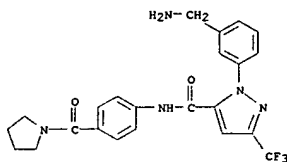
RN 209956-77-4 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209956-78-5 CAPLUS

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



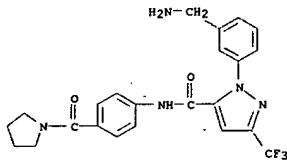
RN 209957-00-6 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209956-99-0

CMF C23 H22 F3 N5 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 209957-27-7 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-4-methoxy-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

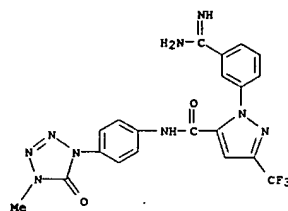
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209956-77-4

CMF C20 H16 F3 N9 O2



CM 2

CRN 76-05-1

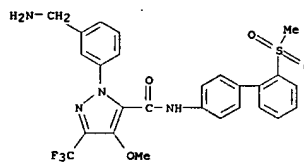
CMF C2 H F3 O2



RN 209956-99-0 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



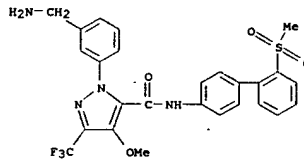
RN 209957-28-8 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-4-methoxy-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-27-7

CMF C26 H23 F3 N4 O4 S



CM 2

CRN 76-05-1

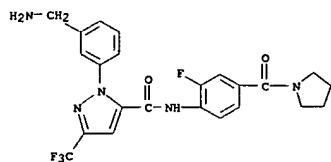
CMF C2 H F3 O2



RN 209957-29-9 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

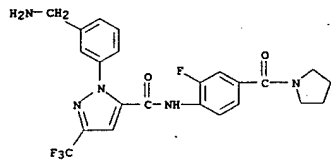


RN 209957-30-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-29-9

CMF C23 H21 F4 N5 O2



CM 2

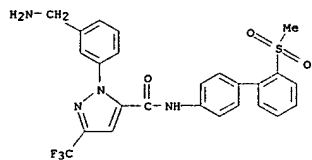
CRN 76-05-1

CMF C2 H F3 O2



RN 209957-31-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

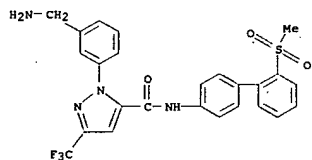


RN 209957-34-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-33-5

CMF C25 H21 F3 N4 O3 S



CM 2

CRN 76-05-1

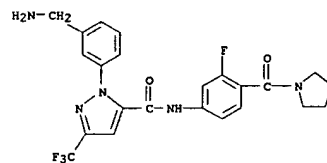
CMF C2 H F3 O2



RN 209957-35-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-(2-(aminosulfonyl)phenyl)-1,4-dihydro-2-pyrimidinyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

10519356a.trn

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

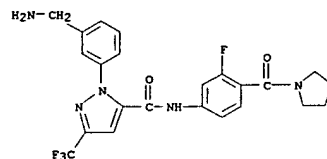


RN 209957-32-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-31-3

CMF C23 H21 F4 N5 O2



CM 2

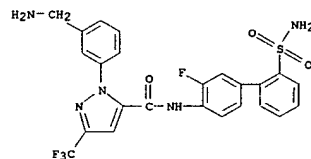
CRN 76-05-1

CMF C2 H F3 O2



RN 209957-33-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

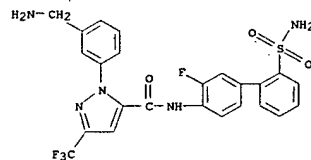


RN 209957-36-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-35-7

CMF C24 H19 F4 N5 O3 S



CM 2

CRN 76-05-1

CMF C2 H F3 O2



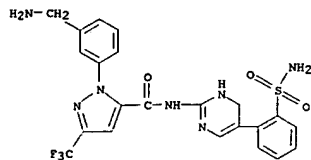
RN 209957-38-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-(2-(aminosulfonyl)phenyl)-1,4-dihydro-2-pyrimidinyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 209957-37-9

CMF C22 H20 F3 N7 O3 S



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 209957-40-4 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-39-1

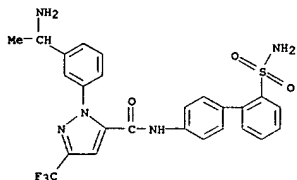
CMF C22 H18 F3 N7 O3 S

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 209957-41-5

CMF C25 H22 F3 N5 O3 S



CM 2

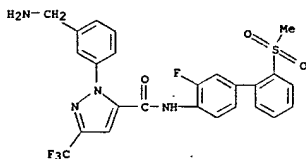
CRN 76-05-1

CMF C2 H F3 O2



RN 209957-47-1 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

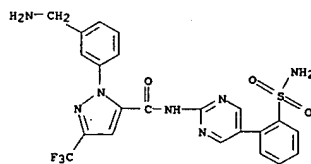


RN 209957-48-2 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

10519356a.trn

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

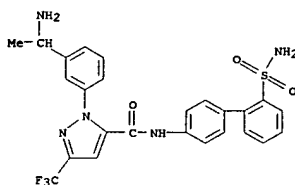
CRN 76-05-1

CMF C2 H F3 O2



RN 209957-41-5 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(1-aminoethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-42-6 CAPLUS

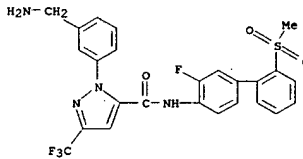
CN 1H-Pyrazole-5-carboxamide, 1-[3-(1-aminoethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 209957-47-1

CMF C25 H20 F4 N4 O3 S



CM 2

CRN 76-05-1

CMF C2 H F3 O2



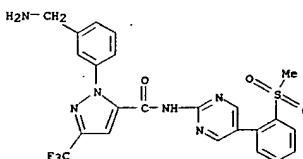
RN 209957-50-6 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

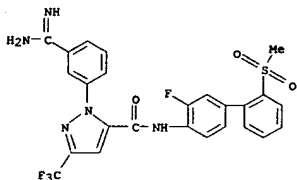
CRN 209957-49-3

CMF C23 H19 F3 N6 O3 S



CM 2

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

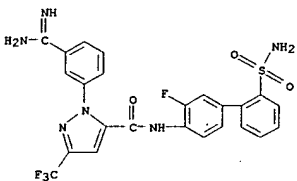
CRN 76-05-1
CMF C2 H F3 O2RN 209957-51-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)RN 209957-52-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

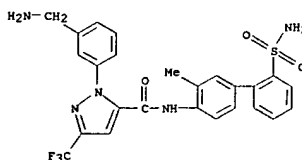
CRN 209957-51-7
CMF C25 H19 F4 N5 O3 S

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

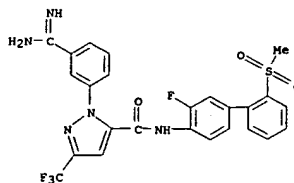
CRN 209957-53-9
CMF C24 H18 F4 N6 O3 S

CM 2

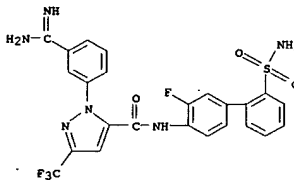
CRN 76-05-1
CMF C2 H F3 O2RN 209957-67-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-methyl[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)RN 209957-68-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-methyl[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

10519356a.trn

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

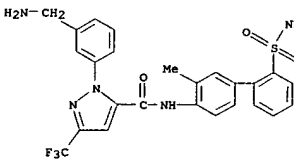


CM 2

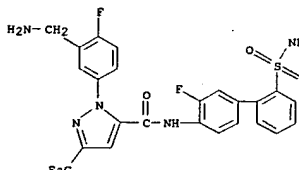
CRN 76-05-1
CMF C2 H F3 O2RN 209957-53-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)RN 209957-54-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 209957-67-5
CMF C25 H22 F3 N5 O3 S

CM 2

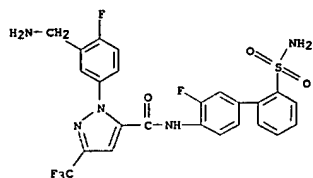
CRN 76-05-1
CMF C2 H F3 O2RN 209957-73-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)RN 209957-74-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 209957-73-3

CMF C24 H18 F5 N5 O3 S



CM 2

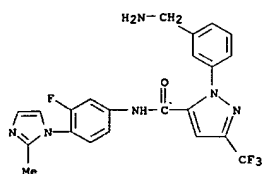
CRN 76-05-1

CMF C2 H F3 O2



RN 209957-83-5 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

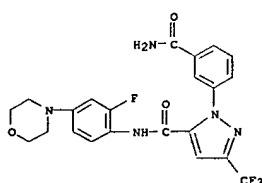


L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



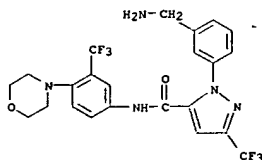
RN 209957-91-5 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-92-6 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(4-morpholinyl)-3-(trifluoromethyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-93-7 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(4-morpholinyl)-3-(trifluoromethyl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

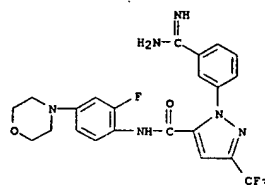
CRN 209957-92-6

CMF C23 H21 F6 N5 O2

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209957-89-1 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-90-4 CAPLUS

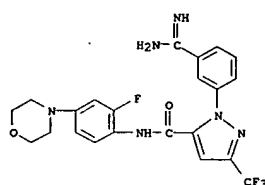
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI)

(CA INDEX NAME)

CM 1

CRN 209957-89-1

CMF C22 H20 F4 N6 O2

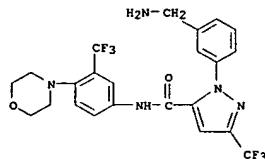


CM 2

CRN 76-05-1

CMF C2 H F3 O2

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

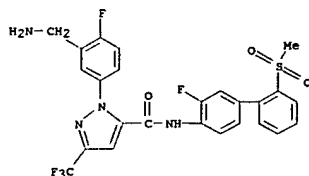
CRN 76-05-1

CMF C2 H F3 O2



RN 209958-13-4 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209958-14-5 CAPLUS

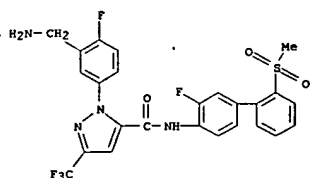
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209958-13-4

CMF C25 H19 F5 N4 O3 S

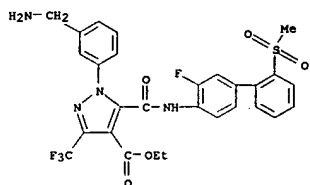
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CH 2
CRN 76-05-1
CHF C2 H F3 O2

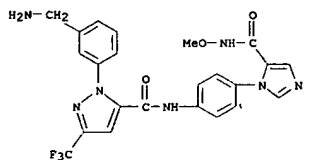


RN 209958-21-4 CAPLUS
CN 1H-Pyrazole-4-carboxylic acid,
1-[3-(aminomethyl)phenyl]-5-[[3-fluoro-2'-(
(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-,
ethyl ester (9CI) (CA INDEX NAME)

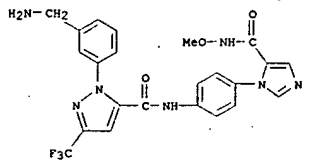


RN 209958-22-5 CAPLUS
CN 1H-Pyrazole-4-carboxylic acid,
1-[3-(aminomethyl)phenyl]-5-[[3-fluoro-2'-(

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209958-29-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[5-
[(methoxyamino)carbonyl]-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)
CH 1
CRN 209958-28-1
CHF C23 H20 F3 N7 O3



CH 2
CRN 76-05-1
CHF C2 H F3 O2

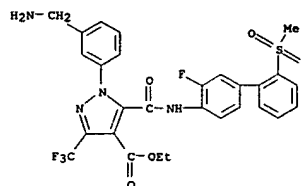


RN 209958-30-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(5-methyl-1H-
1,2,3-triazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-,
ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
CRN 209958-21-4
CHF C28 H24 F4 N4 O5 S

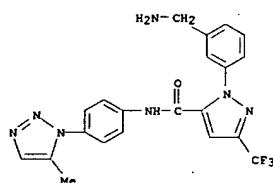


CH 2
CRN 76-05-1
CHF C2 H F3 O2

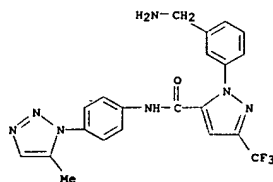


RN 209958-28-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[5-
[(methoxyamino)carbonyl]-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)-
(9CI) (CA INDEX NAME)

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209958-31-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(5-methyl-1H-
1,2,3-triazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate)
(9CI) (CA INDEX NAME)
CH 1
CRN 209958-30-5
CHF C21 H18 F3 N7 O

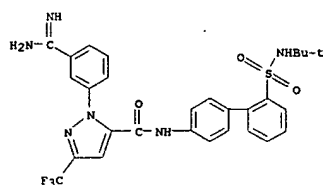


CH 2
CRN 76-05-1
CHF C2 H F3 O2



RN 209958-33-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-[(1,1-
dimethylethyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-

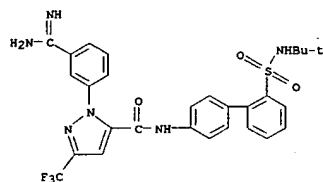
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(9CI) (CA INDEX NAME)



RN 256512-05-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-[[1,1-dimethylethyl]amino]sulfonyl]-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, trifluoroacetate (5:6) (9CI) (CA INDEX NAME)

CM 1

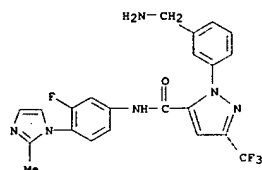
CRN 209958-33-8
CMF C28 H27 F3 N6 O3 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CRN 209957-83-5
CMF C22 H18 F4 N6 O

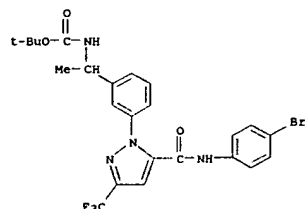


CM 2

CRN 76-05-1
CMF C2 H F3 O2



IT 209960-02-1P
RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of azoles as Factor Xa inhibitors)
RN 209960-02-1 CAPLUS
CN Carbamic acid, [1-[3-[5-[[4-bromophenyl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



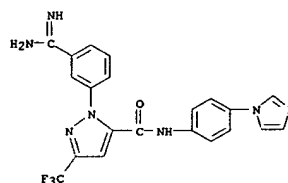
L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 256512-19-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209956-75-2
CMF C21 H16 F3 N7 O



CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 256512-30-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

L9 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

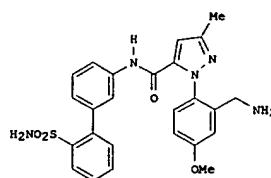
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
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 DOCUMENT NUMBER: 131:58820
 TITLE: Preparation of nitrogen heteroaromatics as blood coagulation factor Xa inhibitors
 INVENTOR(S): Galemmo, Robert A., Jr.; Pinto, Donald J. P.; Bostrom,
 PATENT ASSIGNEE(S): Lori L.; Rossi, Karen Anita
 SOURCE: Du Pont Pharmaceuticals Company, USA
 PCT Int. Appl., 237 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9932454	A1	19990701	WO 1998-US26427	19981211
W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2314401	A1	19990701	CA 1998-2314401	19981211
AU 9917244	A	19990712	AU 1999-17244	19981211
BR 9813835	A	20001010	BR 1998-13835	19981211
EP 1042299	A1	20001011	EP 1998-962082	19981211
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
JP 2001526268	T	20011218	JP 2000-525391	19981211
ZA 9811517	A	20000615	ZA 1998-11517	19981215
US 6271237	B1	20010807	US 1998-217336	19981221
US 2002016326	A1	20020207	US 2001-833302	20010412
US 6548525	B2	20030415		

PRIORITY APPLN. INFO.:
 US 1997-68491P P 19971222
 US 1997-996447 A 19971222
 US 1998-101075P P 19980918
 WO 1998-US26427 W 19981211
 US 1998-217336 A3 19981221

OTHER SOURCE(S): MARPAT 131:58820
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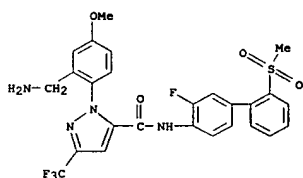
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



II

AB DEG(CH2)4MZAB [I: D = cyano, amino(alkyl), amidino, etc.; E = (un)substituted phenylene, -pyridinediyl, -pyrimidinediyl, etc.; G = bond, NHCH2, OCH2, SCH2; M = (un)substituted pyrrolylene, -di-, -tri-, or -tetrazolylene; Z = (heteroatom-interrupted) (oxo)alkylene, oxyalkylene, alkyleneoxy, etc.; A = (un)substituted carbocyclic residue (sicc) or -heterocyclylene; B = amino(alkyl), amidino, ureido, (un)substituted carbocyclic residue, etc.; s = 0-2] were prepared Thus, 2-hydrazino-5-methoxybenzoic acid was cyclocondensed with MeCOCH2C(=NOMe)CO2Et (preparation each given) and the product converted in 3 steps to 3-methyl-1-(2-azidomethyl-4-methoxyphenyl)-1H-pyrazole-5-carboxylic acid which was amidated by 4-(H2N)C6H4C6H4(CO2NHOMe)-2 to give, in 2 addnl. steps, title compound II. Data for biol. activity of I were given.
 IT 228258-60-4P 228258-89-6P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (Preparation of nitrogen heteroaroms. as blood coagulation factor Xa inhibitors)
 RN 228258-60-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)
 CH 1
 CRN 228257-56-5
 CMF C26 H22 F4 N4 O4 S

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

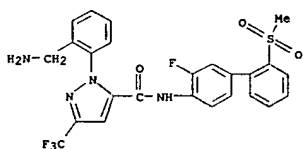


CH 2
 CRN 76-05-1
 CMF C2 H F3 O2



RN 228258-88-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
 CRN 228258-46-6
 CMF C25 H20 F4 N4 O3 S



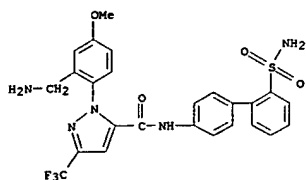
CH 2
 CRN 76-05-1
 CMF C2 H F3 O2

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

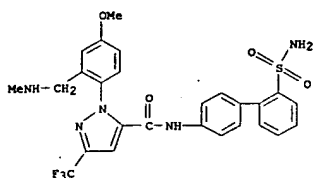


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 228257-65-6P 228257-68-9P 228257-71-4P
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 228258-85-3P 228258-86-4P 228258-87-5P
 228258-88-6P 228258-89-7P 228258-90-8P
 228258-91-9P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (Preparation of nitrogen heteroaroms. as blood coagulation factor Xa inhibitors)
 RN 228257-38-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

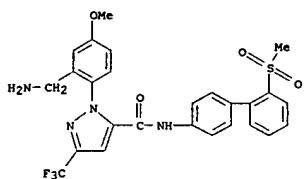
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



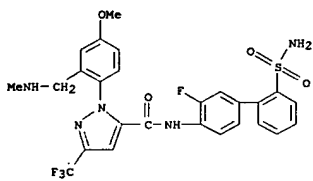
RN 228257-41-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-
methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)



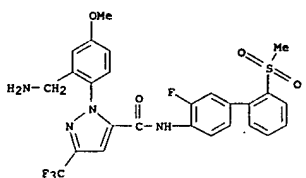
RN 228257-44-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-
(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)



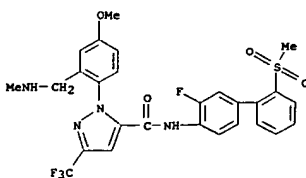
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228257-56-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-(aminomethyl)-4-methoxyphenyl]-N-[3-fluoro-
2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)



RN 228257-59-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-
4-yl]-1-[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)-
(9CI) (CA INDEX NAME)

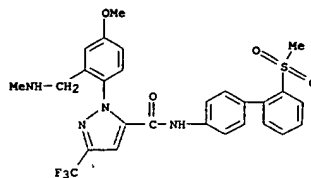


RN 228257-62-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[4-(1-
pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

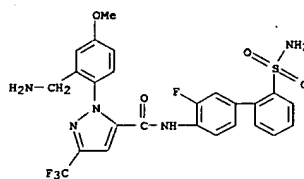
10519356a.trn

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 228257-47-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[4-methoxy-2-[(methylamino)methyl]phenyl]-N-
[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)

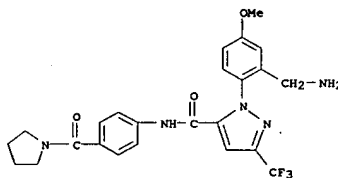


RN 228257-50-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-
(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI)
(CA INDEX NAME)

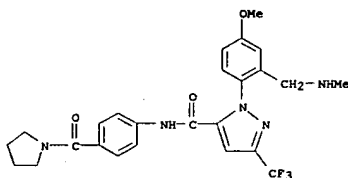


RN 228257-53-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-
yl]-1-[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)-
(9CI) (CA INDEX NAME)

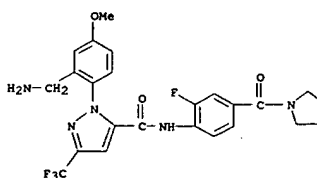
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 228257-65-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[4-methoxy-2-[(methylamino)methyl]phenyl]-N-
[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX
NAME)



RN 228257-68-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide,
1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2-fluoro-
4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX
NAME)

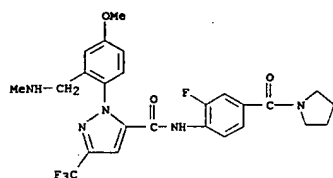


L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 228257-71-4 CAPLUS

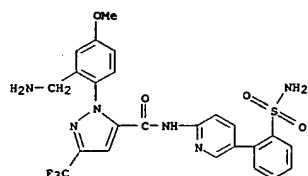
CN 1H-Pyrazole-5-carboxamide.

INDEX NAME) N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-1-[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA



RN 228257-74-7 CAPLUS

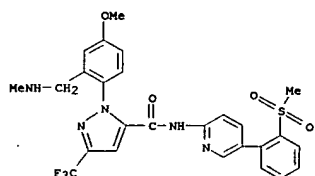
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 228257-77-0 CAPLUS

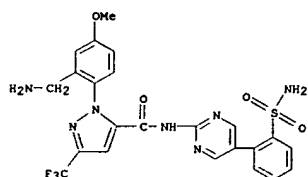
1H-Pyrazole-5-carboxamide, N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-1-[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



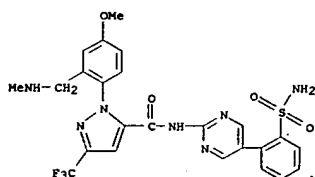
RN 228257-86-1 CAPLUS

1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 228257-89-4 CAPLUS

1H-Pyrazole-5-carboxamide,
N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-1-
[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA
INDEX NAME)

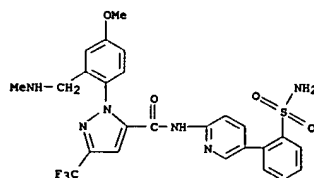


RN 228257-92-9 CAPLUS

220257-52-9 CAPLOS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA

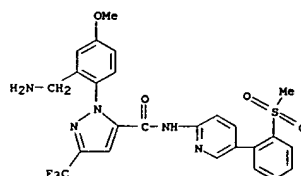
10519356a.trn

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228257-80-5 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[5-(2-(methylsulfonyl)phenyl)-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA
INDEX
NAME)

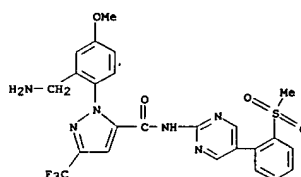


RN 228257-83-8 CAPLUS

1H-Pyrazole-5-carboxamide, 1-[4-methoxy-2-[(methylamino)methyl]phenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI)

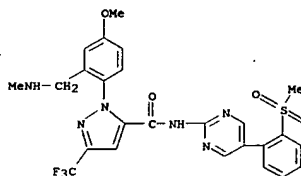
(CA INDEX NAME)

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
INDEX NAME)



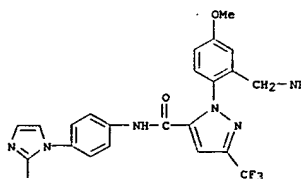
RN 228257-95-2 CAPLUS

1H-Pyrazole-5-carboxamide, 1-[4-methoxy-2-[(methylamino)methyl]phenyl]-N-
[5-[2-(methylsulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI)
(CA INDEX NAME)



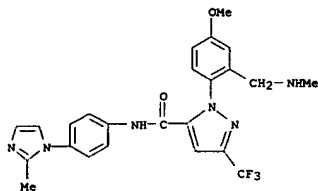
RN 228257-98-5 CAPLUS

CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

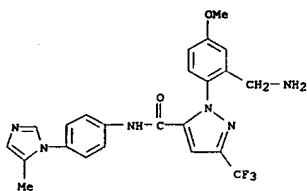


RN 228258-01-3 CAPLUS

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CN 1H-Pyrazole-5-carboxamide, 1-[4-methoxy-2-[(methylamino)methyl]phenyl]-N-[4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



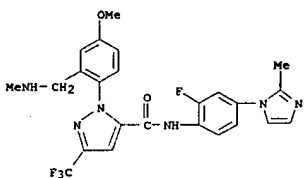
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 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[4-(5-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



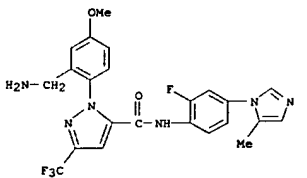
RN 228258-07-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[4-methoxy-2-[(methylamino)methyl]phenyl]-N-[4-(5-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



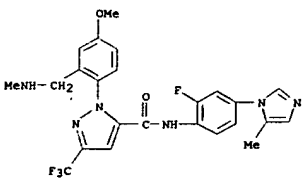
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-16-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2-fluoro-4-(5-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



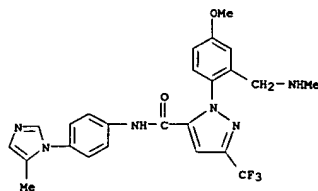
RN 228258-19-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(5-methyl-1H-imidazol-1-yl)phenyl]-1-[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



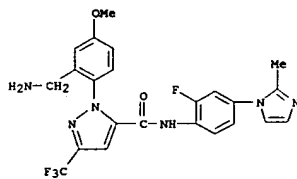
RN 228258-22-8 CAPLUS

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L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



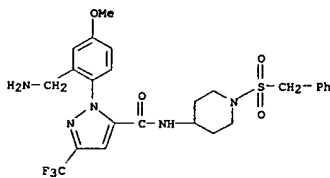
RN 228258-10-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



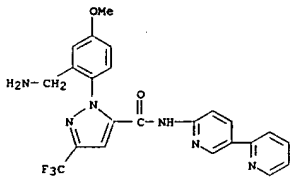
RN 228258-13-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]-1-[4-methoxy-2-[(methylamino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



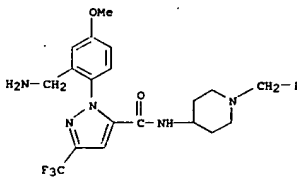
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[1-(phenylmethyl)sulfonyl]-4-piperidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 228258-23-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2,3'-bipyridin]-6'-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

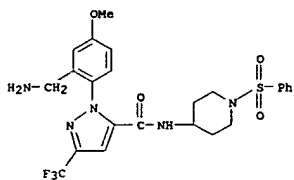


RN 228258-24-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[1-(phenylmethyl)-4-piperidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

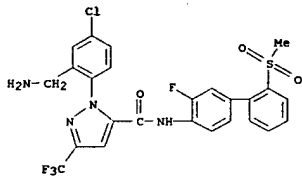


RN 228258-25-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[1-

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 (phenylsulfonyl)-4-piperidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

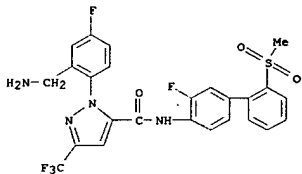


RN 228258-26-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 1-[2-(aminomethyl)-4-chlorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)]-1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

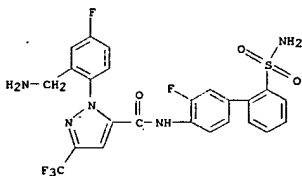


RN 228258-27-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-chlorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

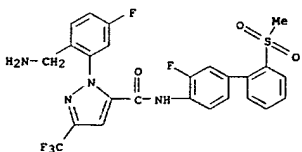
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CN 1H-Pyrazole-5-carboxamide,
 1-[2-(aminomethyl)-4-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)]-1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



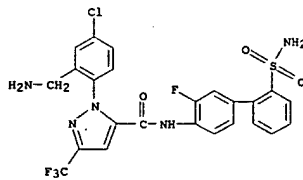
RN 228258-31-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



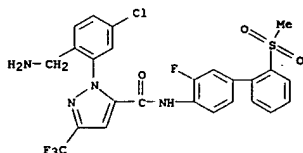
RN 228258-32-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 1-[2-(aminomethyl)-5-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)]-1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



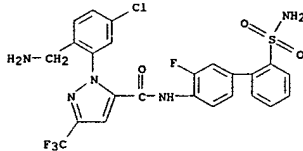
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-28-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 1-[2-(aminomethyl)-5-chlorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)]-1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



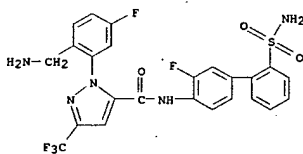
RN 228258-29-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-5-chlorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



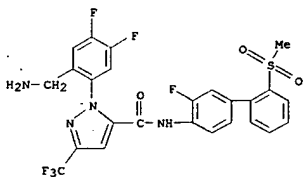
RN 228258-30-8 CAPLUS

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 228258-33-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-5-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

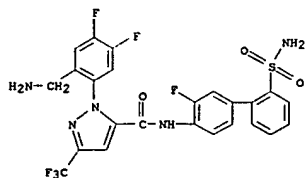


RN 228258-34-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4,5-difluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)]-1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

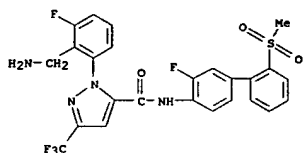


RN 228258-35-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4,5-difluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

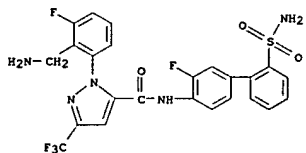
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-36-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-((aminomethyl)-3-fluorophenyl)-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

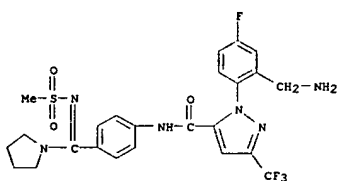


RN 228258-37-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-((aminomethyl)-3-fluorophenyl)-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

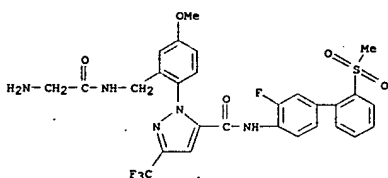


RN 228258-38-6 CAPLUS

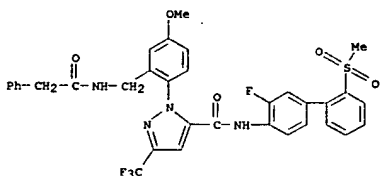
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-41-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-((aminomethyl)phenyl)-4-methoxyphenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



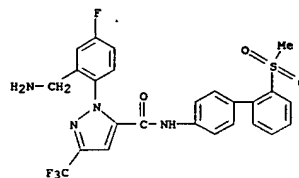
RN 228258-42-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[4-methoxy-2-((phenylacetyl)amino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



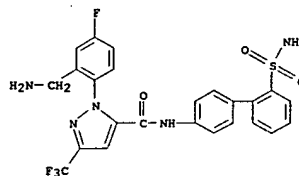
RN 228258-43-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-((aminomethyl)phenyl)-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10519356a.trn

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide, 1-[2-((aminomethyl)-4-fluorophenyl)-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

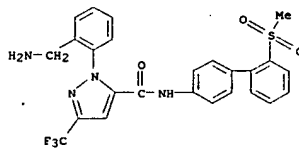


RN 228258-39-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-((aminomethyl)-4-fluorophenyl)-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

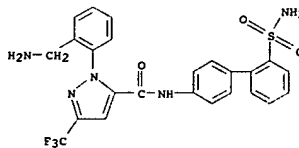


RN 228258-40-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-((aminomethyl)-4-fluorophenyl)-N-[4-[[methylsulfonyl]imino]-1-pyrrolidinylmethyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

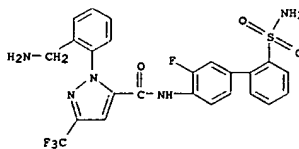
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-5-carboxamide, 1-[2-((aminomethyl)-4-fluorophenyl)-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 228258-44-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-((aminomethyl)phenyl)-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

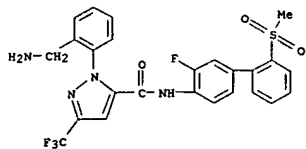


RN 228258-45-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-((aminomethyl)phenyl)-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

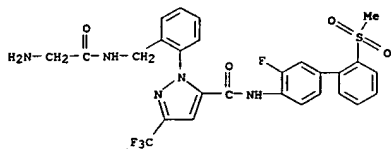


RN 228258-46-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-((aminomethyl)phenyl)-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

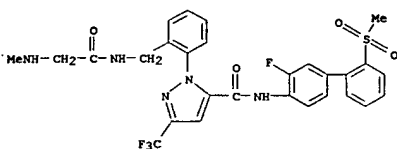
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-47-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-((aminomethyl)amino)methyl]phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 228258-48-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[2-(((methylamino)acetyl)amino)methyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

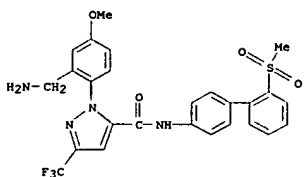


RN 228258-49-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminocarbonyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 (methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228257-44-1
 CMF C26 H23 F3 N4 O4 S



CM 2

CRN 76-05-1
 CMF C2 H F3 O2

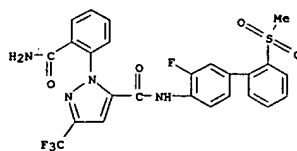


RN 228258-62-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228257-38-3
 CMF C25 H22 F3 N5 O4 S

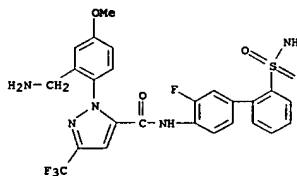
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-59-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228257-50-9
 CMF C25 H21 F4 N5 O4 S



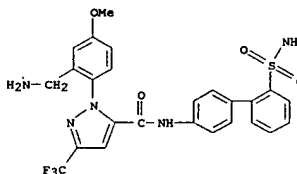
CM 2

CRN 76-05-1
 CMF C2 H F3 O2



RN 228258-61-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

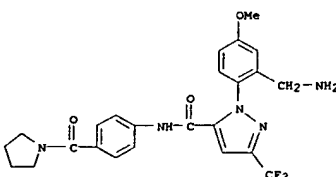
CRN 76-05-1
 CMF C2 H F3 O2



RN 228258-63-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228257-62-3
 CMF C24 H24 F3 N5 O3



CM 2

CRN 76-05-1

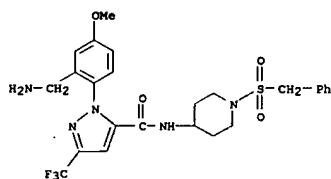
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CNF C2 H F3 O2



RN 228258-64-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[1-(phenylmethyl)sulfonyl]-4-piperidinyl-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 228258-22-8
 CNF C25 H28 F3 N5 O4 S



CH 2

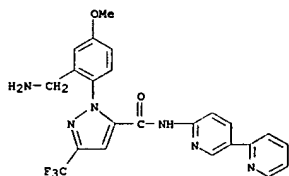
CRN 76-05-1
 CNF C2 H F3 O2



RN 228258-65-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[5-(aminosulfonyl)phenyl]-2-pyridinyl-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CH 2

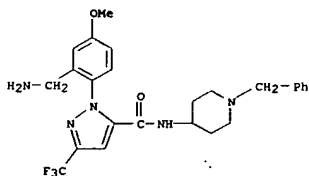
CRN 76-05-1
 CNF C2 H F3 O2



RN 228258-67-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[1-(phenylmethyl)-4-piperidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 228258-24-0
 CNF C25 H28 F3 N5 O2



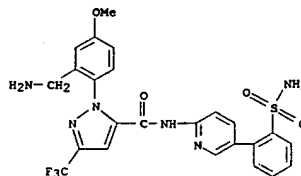
CH 2

CRN 76-05-1

10519356a.trn

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 228257-74-7
 CNF C24 H21 F3 N6 O4 S



CH 2

CRN 76-05-1
 CNF C2 H F3 O2



RN 228258-66-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[2,3'-bipyridin]-6'-yl-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 228258-23-9
 CNF C23 H19 F3 N6 O2

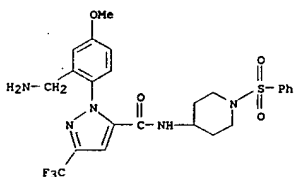
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-68-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[1-(phenylsulfonyl)-4-piperidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 228258-25-1
 CNF C24 H26 F3 N5 O4 S



CH 2

CRN 76-05-1
 CNF C2 H F3 O2

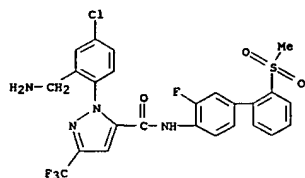


RN 228258-69-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-chlorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)-1,1'-biphenyl]-4-yl-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 228258-26-2
 CNF C25 H19 Cl F4 N4 O3 S

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

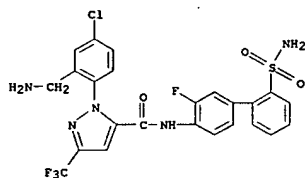


CH 2
CRN 76-05-1
CMF C2 H F3 O2



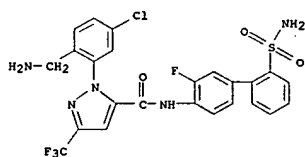
RN 228258-70-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-chlorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
CRN 228258-27-3
CMF C24 H18 Cl F4 N5 O3 S



L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
CRN 228258-29-5
CMF C24 H18 Cl F4 N5 O3 S



CH 2
CRN 76-05-1
CMF C2 H F3 O2



RN 228258-73-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
CRN 228258-30-8
CMF C25 H19 F5 N4 O3 S

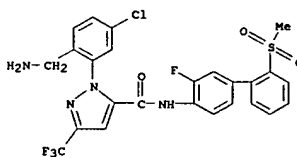
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CH 2
CRN 76-05-1
CMF C2 H F3 O2



RN 228258-71-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-5-chlorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
CRN 228258-28-4
CMF C25 H19 Cl F4 N4 O3 S

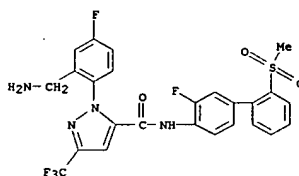


CH 2
CRN 76-05-1
CMF C2 H F3 O2



RN 228258-72-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-5-chlorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

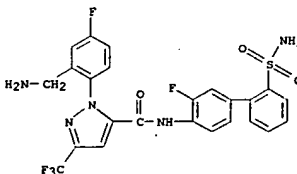


CH 2
CRN 76-05-1
CMF C2 H F3 O2



RN 228258-74-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
CRN 228258-31-9
CMF C24 H18 F5 N5 O3 S



CH 2
CRN 76-05-1
CMF C2 H F3 O2

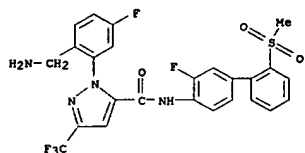
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228258-75-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-5-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-32-0
 CHF C25 H19 F5 N4 O3 S



CM 2

CRN 76-05-1
 CHF C2 H F3 O2



RN 228258-76-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-5-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 2

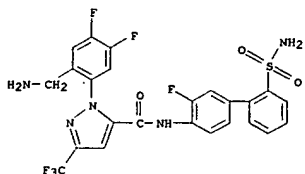
CRN 76-05-1
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RN 228258-78-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4,5-difluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 228258-35-3
 CHF C24 H17 F6 N5 O3 S



CM 2

CRN 76-05-1
 CHF C2 H F3 O2

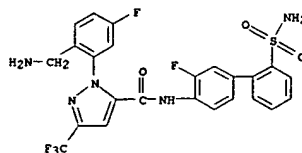


RN 228258-79-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-3-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 228258-33-1
 CHF C24 H18 F5 N5 O3 S



CM 2

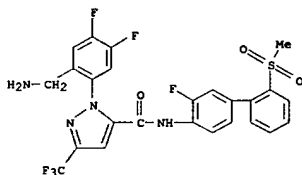
CRN 76-05-1
 CHF C2 H F3 O2



RN 228258-77-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4,5-difluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

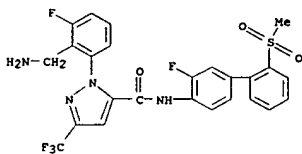
CRN 228258-34-2
 CHF C25 H18 F6 N4 O3 S



L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 228258-36-4
 CHF C25 H19 F5 N4 O3 S



CM 2

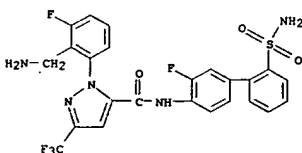
CRN 76-05-1
 CHF C2 H F3 O2



RN 228258-80-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-3-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

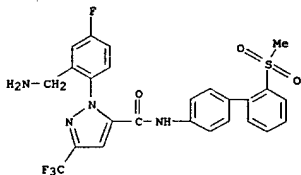
CRN 228258-37-5
 CHF C24 H18 F5 N5 O3 S



L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CM 2
 CRN 76-05-1
 CMF C2 H F3 O2



RN 228258-81-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)
 CM 1
 CRN 228258-38-6
 CMF C25 H20 F4 N4 O3 S

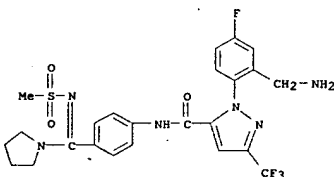


CM 2
 CRN 76-05-1
 CMF C2 H F3 O2



RN 228258-82-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-,

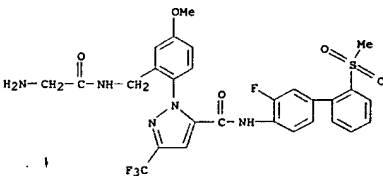
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2
 CRN 76-05-1
 CMF C2 H F3 O2



RN 228258-84-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[aminoacetyl]amino]methyl]-4-methoxyphenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)
 CM 1
 CRN 228258-41-1
 CMF C28 H25 F4 N5 O5 S

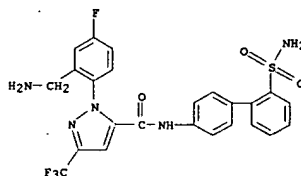


CM 2
 CRN 76-05-1

10519356a.trn

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1
 CRN 228258-39-7
 CMF C24 H19 F4 N5 O3 S



CM 2
 CRN 76-05-1
 CMF C2 H F3 O2



RN 228258-83-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-fluorophenyl]-N-[4-[[[methylsulfonyl]imino]-1-pyrrolidinylmethyl]phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

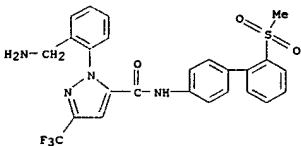
CM 1
 CRN 228258-40-0
 CMF C24 H24 F4 N6 O3 S

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CMF C2 H F3 O2



RN 228258-85-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1
 CRN 228258-43-3
 CMF C25 H21 F3 N4 O3 S



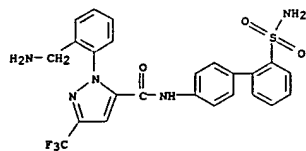
CM 2
 CRN 76-05-1
 CMF C2 H F3 O2



RN 228258-86-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1
 CRN 228258-44-4
 CMF C24 H20 F3 N5 O3 S

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

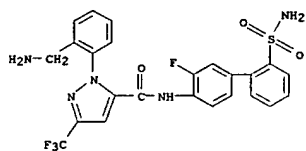


CM 2
CRN 76-05-1
CHF C2 H F3 O2



RN 228258-87-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

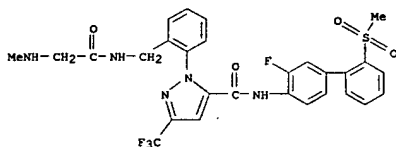
CM 1
CRN 228258-45-5
CHF C24 H19 F4 N5 O3 S



CM 2

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 228258-48-8
CHF C28 H25 F4 N5 O4 S

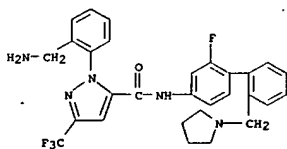


CM 2
CRN 76-05-1
CHF C2 H F3 O2



RN 228258-99-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2-fluoro-2'-(1-pyrrolidinylmethyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1
CRN 228258-98-8
CHF C29 H27 F4 N5 O



CM 2
CRN 76-05-1

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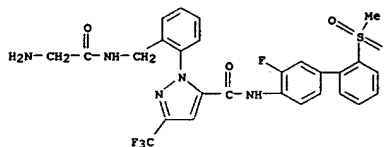
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 76-05-1
CHF C2 H F3 O2



RN 228258-89-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-[[[aminoacetyl]amino]methyl]phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1
CRN 228258-47-7
CHF C27 H23 F4 N5 O4 S



CM 2
CRN 76-05-1
CHF C2 H F3 O2



RN 228258-90-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-1-[2-[[[methylamino]acetyl]amino]methyl]phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

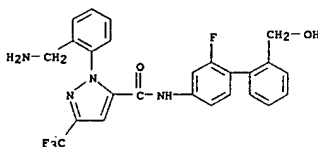
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CHF C2 H F3 O2



RN 228259-01-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)phenyl]-N-[2-fluoro-2'-(hydroxymethyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1
CRN 228259-00-5
CHF C25 H20 F4 N4 O2

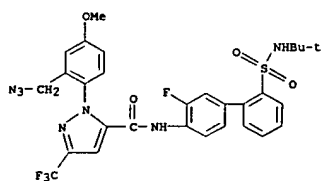


CM 2
CRN 76-05-1
CHF C2 H F3 O2

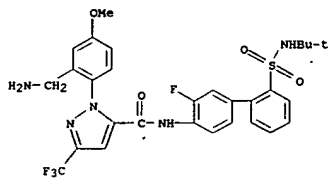


IT 228259-20-9P 228259-21-0P 228259-22-1P
228259-23-2P 228259-24-3P 228259-25-4P
228259-29-6P 228259-36-7P 228259-37-8P
228259-38-9P 228259-39-0P 228259-68-5P
228259-69-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrogen heteroaroms. as blood coagulation factor Xa inhibitors)
RN 228259-20-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(azidomethyl)-4-methoxyphenyl]-N-[2'-[[[1,1-dimethylethyl]amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]-3-

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(trifluoromethyl)-(9CI) (CA INDEX NAME)

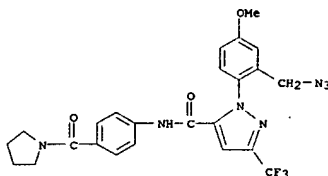


RN 228259-21-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(aminomethyl)-4-methoxyphenyl]-N-[(1,1-dimethylethyl)amino]sulfonyl-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)

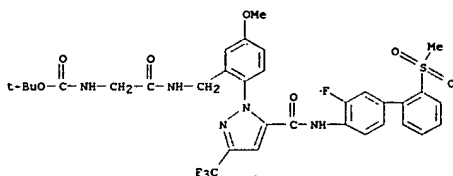


RN 228259-22-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(azidomethyl)-4-methoxyphenyl]-N-[(1,1-dimethylethyl)amino]sulfonyl-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)

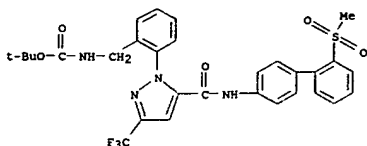
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 228259-25-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(azidomethyl)-4-methoxyphenyl]-N-[(1,1-dimethylethyl)amino]sulfonyl-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)



RN 228259-29-8 CAPLUS
CN Carbamic acid, [(2-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]-5-methoxyphenyl)methyl]amino-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

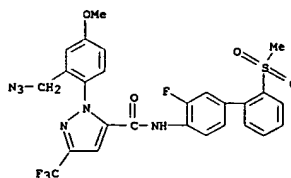


RN 228259-36-7 CAPLUS
CN Carbamic acid, [(2-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]-5-methoxyphenyl)methyl]amino-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

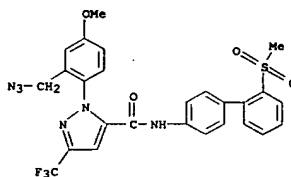


10519356a.trn

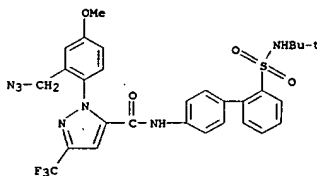
L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 228259-23-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(azidomethyl)-4-methoxyphenyl]-N-[(1,1-dimethylethyl)amino]sulfonyl-3-(trifluoromethyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)

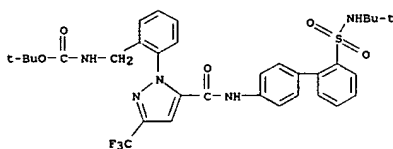


RN 228259-24-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[2-(azidomethyl)-4-methoxyphenyl]-N-[(1,1-dimethylethyl)amino]sulfonyl-3-(trifluoromethyl)-[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)

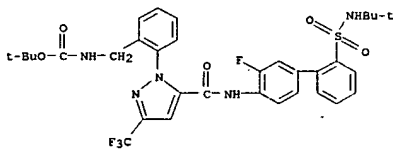


L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

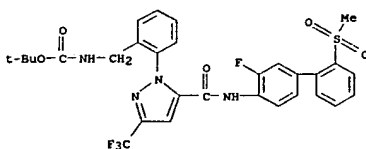
RN 228259-37-8 CAPLUS
CN Carbamic acid, [(2-[5-[[[2'-[[[1,1-dimethylethyl]amino]sulfonyl][1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl)methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 228259-38-9 CAPLUS
CN Carbamic acid, [(2-[5-[[[2'-[[[1,1-dimethylethyl]amino]sulfonyl]-3-fluoro[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl)methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

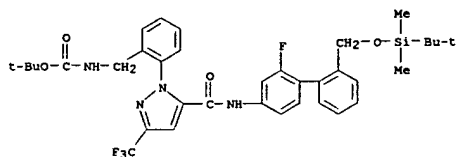


RN 228259-39-0 CAPLUS
CN Carbamic acid, [(2-[5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl)methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

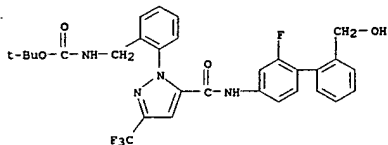


RN 228259-68-5 CAPLUS
CN Carbamic acid, [(2-[5-[[[2'-[[[1,1-dimethylethyl]dimethylsilyl]oxy]methyl]-3-fluoro[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl)methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L9 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
1-2-fluoro[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl)methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 228259-69-6 CAPLUS
CN Carbamic acid, [[2-{5-[[[2-fluoro-2'-(hydroxymethyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl)methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



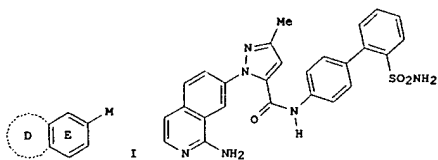
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L9 ANSWER 35 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:9833 CAPLUS
DOCUMENT NUMBER: 130:66494
TITLE: Preparation of novel guanidine mimics as factor Xa inhibitors
INVENTOR(S): Lam, Patrick Y.; Clark, Charles G.; Dominguez, Celia; Fevig, John Matthew; Han, Qi; Li, Renhua; Pinto, Donald Joseph-Phillip; Pruitt, James Russell; Quan, Mimi Lifan
PATENT ASSIGNEE(S): The Du Pont Merck Pharmaceutical Company, USA
SOURCE: PCT Int. Appl., 268 pp.
CODEN: PIXXDZ
LANGUAGE: Patent
English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9857951	A1	19981223	WO 1998-US12680	19980618
W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
ZA 9805247	A	19991217	ZA 1998-5247	19980617
CA 2291442	A1	19981223	CA 1998-2291442	19980618
AU 9879768	A	19990104	AU 1998-79768	19980618
AU 756755	B2	20030123		
EP 991638	A1	20000412	EP 1998-930361	19980618
EP 991638	B1	20050817		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
BR 9810137	A	20000808	BR 1998-10137	19980618
EE 9900583	A	20000815	EE 1999-583	19980618
EE 4153	B1	20031015		
HU 200002686	A2	20020128	HU 2000-2686	19980618
JP 2002505686	T	20020219	JP 1999-504785	19980618
NZ 502370	A	20021025	NZ 1998-502370	19980618
AT 302198	T	20050915	AT 1998-930361	19980618
ES 2244064	T3	20051201	ES 1998-930361	19980618
RO 120543	B1	20060330	RO 1999-1317	19980618
TW 544453	B	20030801	TW 1998-87109910	19980819
NO 9905965	A	19991203	NO 1999-5965	19991203
NO 318359	B1	20050307		
MX 9911908	A	20000531	MX 1999-11908	19991216
LV 12496	B	20010120	LV 1999-178	19991216
LT 4705	B	20000925	LT 1999-147	19991217
PRIORITY APPLN. INFO.:			US 1997-878884	A 19970619
			WO 1998-US12680	W 19980618

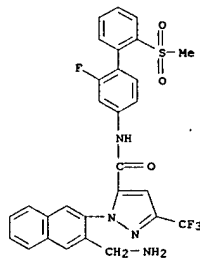
OTHER SOURCE(S): MARPAT 130:66494
GI

L9 ANSWER 35 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

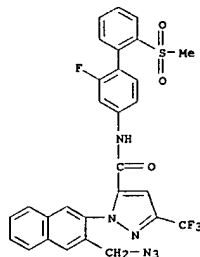


AB The title compds. [I; rings D-E represent guanidine mimics; ring D = CH2N:CH, CH2CH2N:CH, a 5-6 membered aromatic system containing 0-2 heteroatoms selected from the group N, O, and S; ring E is substituted with 0-2 R (substituents), provided that when ring D is unsubstituted, it contains at least one heteroatom; ring E contains 0-2 N atom and is substituted by 0-1 R; R = halo, OH, Cl-3 alkoxy, etc.; M = (un)substituted pyrazole, imidazole, tetrazole, etc.), inhibitors of factor Xa which are useful in treating and preventing a thromboembolic disorder, were prepared and formulated. Thus, a multi-step synthesis of the title compound II, starting with 7-aminoisoquinoline, was described. A number of compds. I were found to exhibit a Ki of $\leq 15 \mu\text{M}$ against factor Xa.
IT 218299-04-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of novel guanidine mimics as factor Xa inhibitors)
RN 218299-04-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-2-naphthalenyl]-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 35 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 218302-16-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of novel guanidine mimics as factor Xa inhibitors)
RN 218302-16-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(azidomethyl)-2-naphthalenyl]-N-[2-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



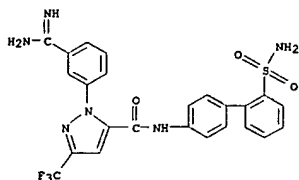
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1998:479506 CAPLUS
 DOCUMENT NUMBER: 129:109090
 TITLE: Preparation of nitrogen-containing heteroaromatics as factor Xa inhibitors
 INVENTOR(S): Pinto, Donald Joseph Phillip; Pruitt, James Russell; Cacciola, Joseph; Fevig, John Matthew; Han, Qi;
 ORwat.
 Michael James; Quan, Mimi Lifan; Rossi, Karen Anita
 PATENT ASSIGNEE(S): The Dupont Merck Pharmaceutical Co., USA
 SOURCE: PCT Int. Appl., 438 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9828269	A1	19980702	WO 1997-US22895	19971215
W: AM, AU, AZ, BR, BY, CA, CN, CZ, EE, HU, IL, JP, KG, KR, KZ, LT, LV, MD, MK, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, UA, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2275796	A1	19980702	CA 1997-2275796	19971215
AU 9856020	A	19980717	AU 1998-56020	19971215
AU 730224	B2	20010301		
EP 946508	A1	19991006	EP 1997-952409	19971215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
EE 9900316	A	20000215	EE 1999-316	19971215
SI 20017	A	20000229	SI 1997-20082	19971215
CN 1246847	A	20000308	CN 1997-181852	19971215
BR 9714073	A	20000509	BR 1997-14073	19971215
HU 200000735	A2	20010428	HU 2000-735	19971215
JP 2001509145	T	20010710	JP 1998-528845	19971215
ZA 9711586	A	19990701	ZA 1997-11586	19971223
TW 492971	B	20020701	TW 1997-86119637	19980203
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MX 9905878	A	20000131	MX 1999-5878	19990622
LT 4673	B	20000725	LT 1999-76	19990622
LV 12430	B	20000720	LV 1999-99	19990730
PRIORITY APPLN. INFO.:			US 1996-769859	A 19961223
			US 1997-879944	A 19970620
			WO 1997-US22895	W 19971215

OTHER SOURCE(S): MARPAT 129:109090
 GI

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 209957-41-5P 209957-42-6P 209957-47-1P
 209957-48-2P 209957-49-3P 209957-50-6P
 209957-51-7P 209957-52-8P 209957-53-9P
 209957-54-0P 209957-57-5P 209957-68-6P
 209957-73-3P 209957-74-4P 209957-83-5P
 209957-84-6P 209957-89-1P 209957-90-4P
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 209958-22-5P 209958-28-1P 209958-29-2P
 209958-30-5P 209958-31-6P 209958-33-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of nitrogen-contg. heteroaroms. as factor Xa inhibitors)
 RN 209954-60-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoininomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)
 CM 1
 CRN 209954-59-6
 CMF C24 H19 F3 N6 O3 S



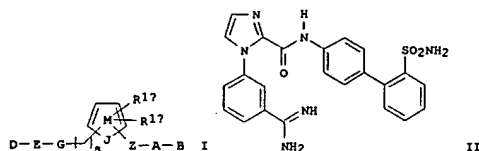
CM 2

CRN 76-05-1
 CMF C2 H F3 O2



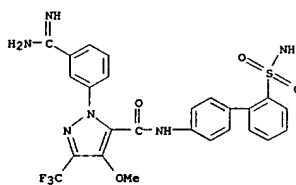
RN 209954-61-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoininomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-4-methoxy-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB The title compds. [I; ring M contains, in addition to J, 0-3 N atoms; J = N, NH; D = CN, C(NR8)NR7R9, C(O)NR7R8, etc.; E = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; DEG = R-substituted pyridyl; R = H, halo, CF3, etc.; G = absent, NHCH2, OCH2, etc.; Z = Cl-4 alkylene, (CH2)nO(CH2)r, etc.; R1a, R1b = absent, NMe, OMe, etc.; A = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S; B = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S, etc.; R7 = H, OH, Cl-6 alkyl, etc.; R8, R9 = H, Cl-6 alkyl, (CH2)nPh; n = 0-3; r = 0-3; s = 0-2], useful as inhibitors of factor Xa, were prepared and formulated. Thus, treatment of 4-[(tert-BuSO2)phenyl]aniline with Me3Al/hexane in CH2Cl2 followed by the addition of Me 1-(3-cyanophenyl)imidazol-2-ylcarboxylate (preparation described), and the Pinner reaction of the resulting intermediate afforded the title compound II. A number of compds. I were found to exhibit a Ki of ≤ 10 μM against factor Xa. Some compds. I were evaluated and found to exhibit Ki of < 10 μM against thrombin.
 IT 209954-60-9P 209954-61-0P 209954-62-1P
 209954-94-9P 209954-95-0P 209954-96-1P
 209955-26-0P 209955-27-1P 209955-28-2P
 209955-36-2P 209955-37-3P 209955-38-4P
 209955-39-5P 209955-40-8P 209955-41-9P
 209955-44-2P 209955-45-3P 209955-46-4P
 209955-47-5P 209955-48-6P 209955-49-7P
 209955-50-0P 209955-51-1P 209955-52-2P
 209955-53-3P 209955-60-2P 209955-61-3P
 209956-54-7P 209956-55-8P 209956-70-7P
 209956-71-8P 209956-75-2P 209956-76-3P
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 209957-29-9P 209957-30-2P 209957-31-3P
 209957-32-4P 209957-33-5P 209957-34-6P
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 209957-38-0P 209957-39-1P 209957-40-4P

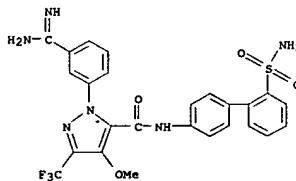
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209954-62-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoininomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-4-methoxy-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209954-61-0
 CMF C25 H21 F3 N6 O4 S



CM 2

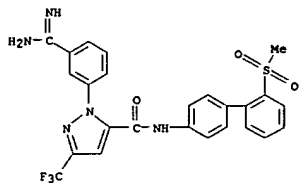
CRN 76-05-1
 CMF C2 H F3 O2



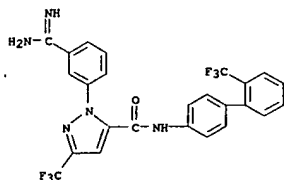
RN 209954-94-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoininomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-4-methoxy-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

.10519356a.trn

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

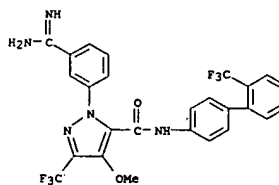


RN 209954-95-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-3-(trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]- (9CI)
(CA INDEX NAME)

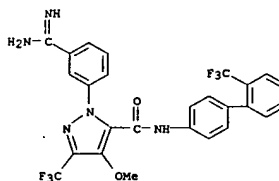


RN 209954-96-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-4-methoxy-3-(trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]- (9CI)
(CA INDEX NAME)

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209955-26-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-4-methoxy-3-(trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)
CH 1
CRN 209954-96-1
CMF C26 H19 F6 N5 O2



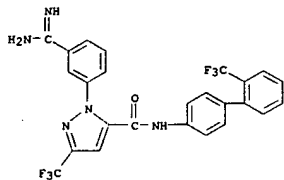
CH 2
CRN 76-05-1
CMF C2 H F3 O2



L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209955-27-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-3-(trifluoromethyl)-N-[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
CRN 209954-95-0
CMF C25 H17 F6 N5 O



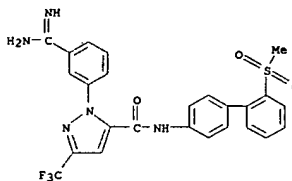
CH 2
CRN 76-05-1
CMF C2 H F3 O2



RN 209955-28-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
CRN 209954-94-9
CMF C25 H20 F3 N5 O3 S

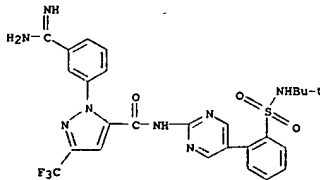
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CH 2
CRN 76-05-1
CMF C2 H F3 O2



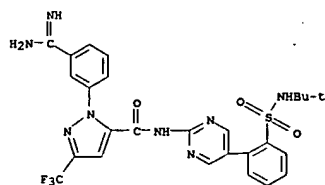
RN 209955-36-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-(2-[[[1,1-dimethylethyl]amino]sulfonyl]phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209955-37-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-(2-[[[1,1-dimethylethyl]amino]sulfonyl]phenyl)-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
CRN 209955-36-2

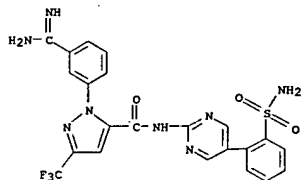
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CNF C26 H23 F3 N8 O3 S



CM 2
 CRN 76-05-1
 CNF C2 H F3 O2

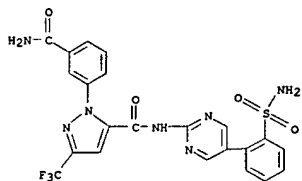


RN 209955-38-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



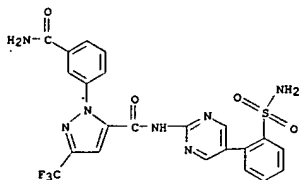
RN 209955-39-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209955-41-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, trifluoroacetate (2:1) (9CI) (CA INDEX NAME)

CM 1
 CRN 209955-40-8
 CNF C22 H16 F3 N7 O4 S



CM 2
 CRN 76-05-1
 CNF C2 H F3 O2



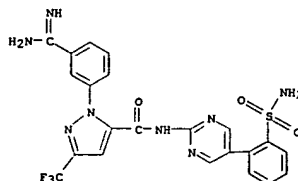
RN 209955-44-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10519356a.trn

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 (aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-38-4
 CNF C22 H17 F3 N8 O3 S

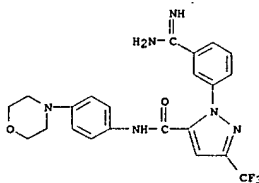


CM 2
 CRN 76-05-1
 CNF C2 H F3 O2



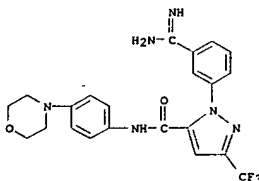
RN 209955-40-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209955-45-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1
 CRN 209955-44-2
 CNF C22 H21 F3 N6 O2

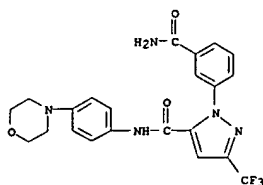


CM 2
 CRN 76-05-1
 CNF C2 H F3 O2



RN 209955-46-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(4-

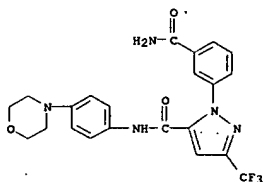
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209955-47-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-46-4
CMF C22 H20 F3 N5 O3



CM 2

CRN 76-05-1
CMF C2 H F3 O2

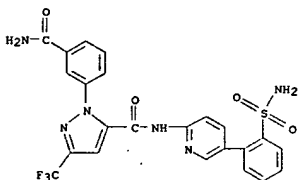
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 209955-50-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209955-51-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

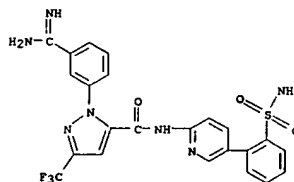
CM 1

CRN 209955-50-0
CMF C23 H17 F3 N6 O4 S

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



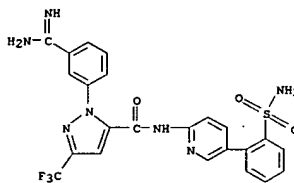
RN 209955-48-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



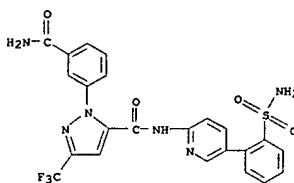
RN 209955-49-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyridinyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-48-6
CMF C23 H18 F3 N7 O3 S



L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

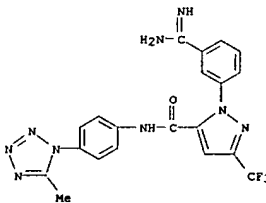


CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 209955-52-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5-methyl-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

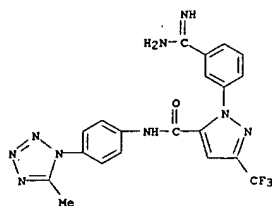


RN 209955-53-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(5-methyl-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209955-52-2

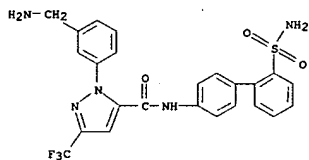
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C20 H16 F3 N5 O



CM 2
CRN 76-05-1
CMF C2 H F3 O2



RN 209955-60-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

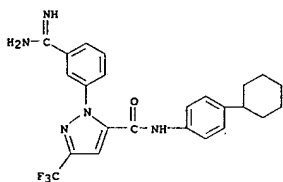


RN 209955-61-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209956-55-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-(4-cyclohexylphenyl)-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1
CRN 209956-54-7
CMF C24 H24 F3 N5 O



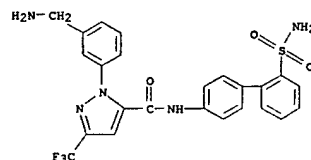
CM 2
CRN 76-05-1
CMF C2 H F3 O2



RN 209956-70-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-chloro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

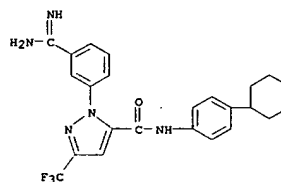
CM 1
CRN 209955-60-2
CMF C24 H20 F3 N5 O3 S



CM 2
CRN 76-05-1
CMF C2 H F3 O2



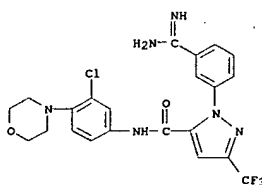
RN 209956-54-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-(4-cyclohexylphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209956-71-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-chloro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1
CRN 209956-70-7
CMF C22 H20 Cl F3 N6 O2

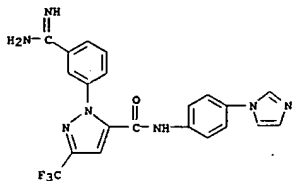


CM 2
CRN 76-05-1
CMF C2 H F3 O2



RN 209956-75-2 CAPLUS

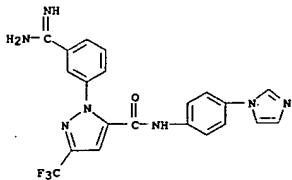
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209956-76-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

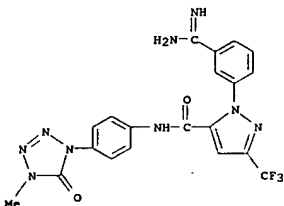
CRN 209956-75-2
 CMF C21 H16 F3 N7 O



CH 2

CRN 76-05-1
 CMF C2 H F3 O2

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

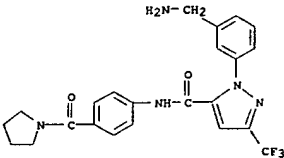


CH 2

CRN 76-05-1
 CMF C2 H F3 O2



RN 209956-99-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-00-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

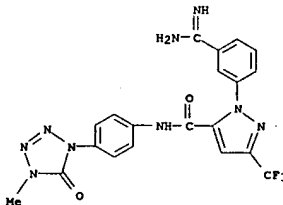
CRN 209956-99-0
 CMF C23 H22 F3 N5 O2

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L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209956-77-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

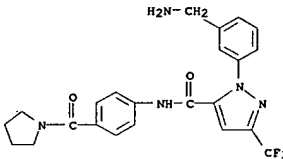


RN 209956-78-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 209956-77-4
 CMF C20 H16 F3 N9 O2

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

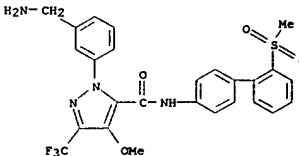


CH 2

CRN 76-05-1
 CMF C2 H F3 O2



RN 209957-27-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-4-methoxy-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

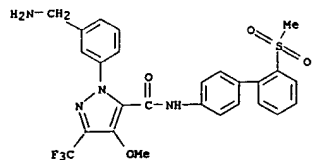


RN 209957-28-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-4-methoxy-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 209957-27-7
 CMF C26 H23 F3 N4 O4 S

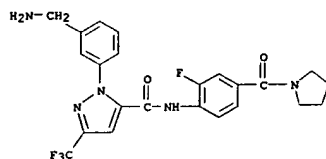
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CH 2
CRN 76-05-1
CHF C2 H F3 O2



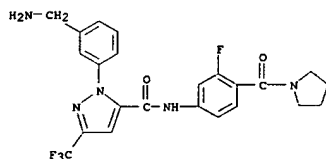
RN 209957-29-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-30-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
CRN 209957-29-9
CHF C23 H21 F4 N5 O2

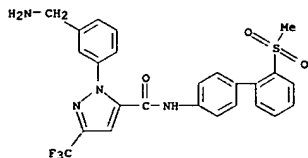
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CH 2
CRN 76-05-1
CHF C2 H F3 O2



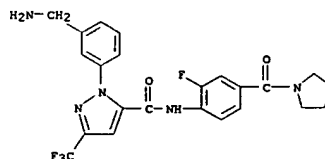
RN 209957-33-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-34-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
CRN 209957-33-5
CHF C25 H21 F3 N4 O3 S

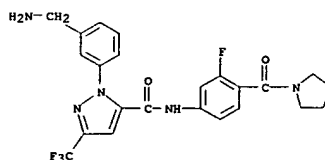
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CH 2
CRN 76-05-1
CHF C2 H F3 O2



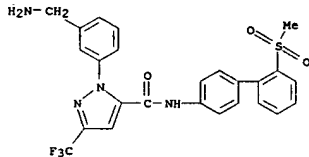
RN 209957-31-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-32-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(1-pyrrolidinylcarbonyl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
CRN 209957-31-3
CHF C23 H21 F4 N5 O2

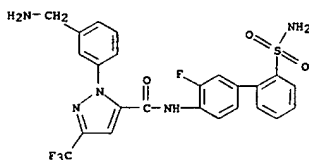
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CH 2
CRN 76-05-1
CHF C2 H F3 O2



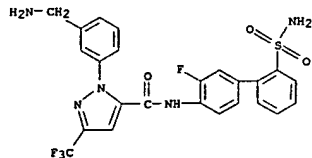
RN 209957-35-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-36-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1
CRN 209957-35-7
CHF C24 H19 F4 N5 O3 S

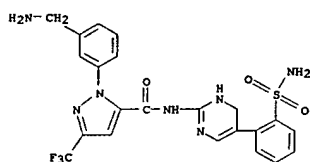
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CHF C2 H F3 O2

RN 209957-37-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-1,4-dihydro-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

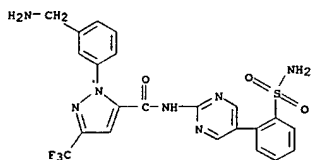


RN 209957-38-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-1,4-dihydro-2-pyrimidinyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-37-9
CHF C22 H20 F3 N7 O3 S

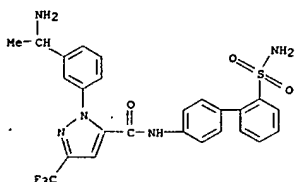
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 209957-39-1
CHF C22 H18 F3 N7 O3 S

CM 2

CRN 76-05-1
CHF C2 H F3 O2

RN 209957-41-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(1-aminoethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

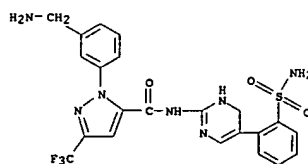


RN 209957-42-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(1-aminoethyl)phenyl]-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

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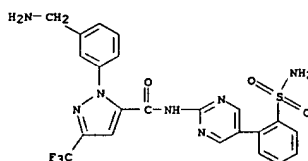
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 76-05-1
CHF C2 H F3 O2

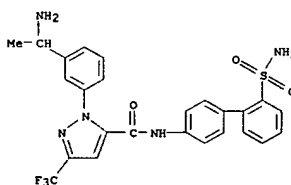
RN 209957-39-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-40-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(aminosulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

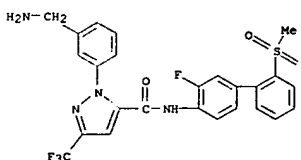
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 209957-41-5
CHF C25 H22 F3 N5 O3 S

CM 2

CRN 76-05-1
CHF C2 H F3 O2

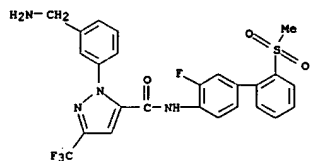
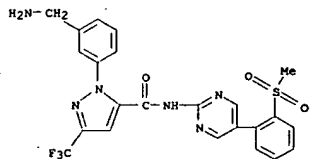
RN 209957-47-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



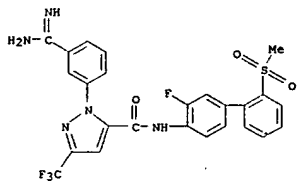
RN 209957-48-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

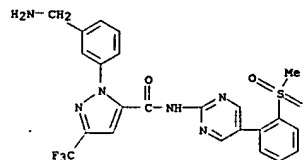
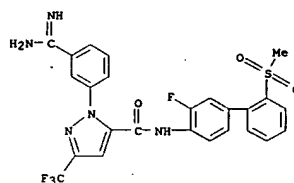
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 209957-47-1
CHF C25 H20 F4 N4 O3 SCM 2
CRN 76-05-1
CHF C2 H F3 O2RN 209957-49-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)RN 209957-50-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[5-[2-(methylsulfonyl)phenyl]-2-pyrimidinyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

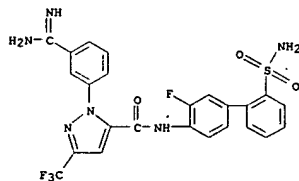
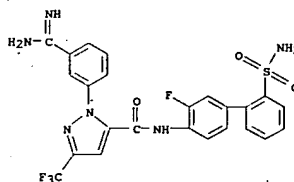
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209957-52-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)CM 1
CRN 209957-51-7
CHF C25 H19 F4 N5 O3 SCM 2
CRN 76-05-1
CHF C2 H F3 O2RN 209957-53-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

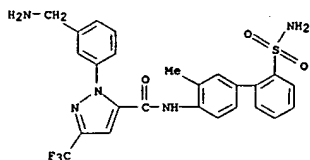
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1
CRN 209957-49-3
CHF C23 H19 F3 N6 O3 SCM 2
CRN 76-05-1
CHF C2 H F3 O2RN 209957-51-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209957-54-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)CM 1
CRN 209957-53-9
CHF C24 H18 F4 N6 O3 SCM 2
CRN 76-05-1
CHF C2 H F3 O2RN 209957-67-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-

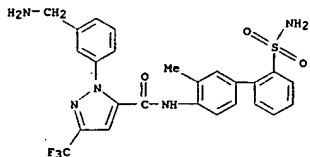
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
3-methyl[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-68-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2'-(aminosulfonyl)-3-methyl[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate)
(9CI) (CA INDEX NAME)

CM 1

CRN 209957-67-5
CMF C25 H22 F3 N5 O3 S



CM 2

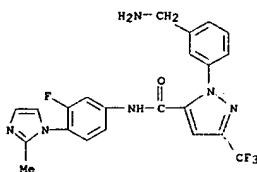
CRN 76-05-1
CMF C2 H F3 O2



L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



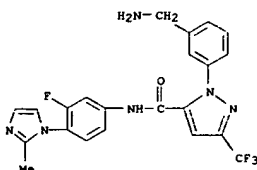
RN 209957-83-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-84-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[3-fluoro-4-(2-methyl-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-83-5
CMF C22 H18 F4 N6 O



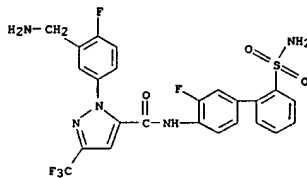
CM 2

CRN 76-05-1
CMF C2 H F3 O2

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L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

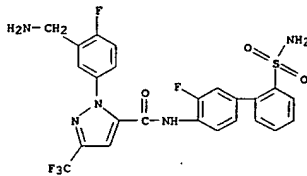
RN 209957-73-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-74-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[2'-(aminosulfonyl)-3-fluoro[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209957-73-3
CMF C24 H18 F5 N5 O3 S



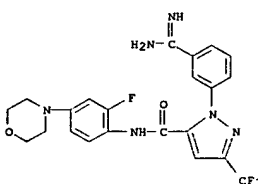
CM 2

CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



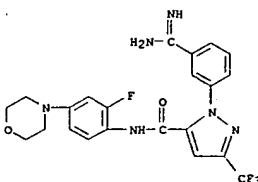
RN 209957-89-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209957-90-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[2-fluoro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

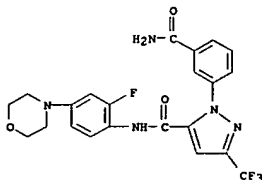
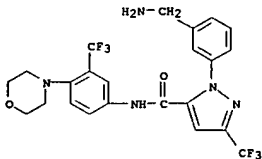
CM 1

CRN 209957-89-1
CMF C22 H20 F4 N6 O2



CM 2

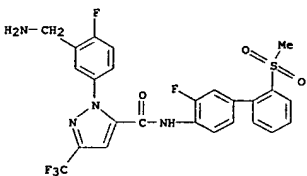
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 76-05-1
CMF C2 H F3 O2RN 209957-91-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[2-fluoro-4-(4-morpholinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)RN 209957-92-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(4-morpholinyl)-3-(trifluoromethyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)RN 209957-93-7 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(4-morpholinyl)-3-(trifluoromethyl)phenyl]-3-(trifluoromethyl)-, bis(trifluoroacetate)

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209958-14-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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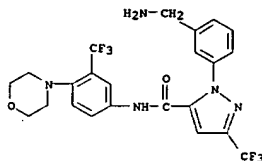
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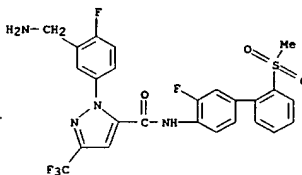
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L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

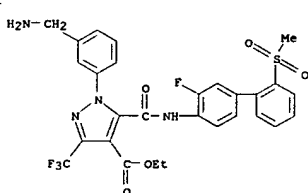
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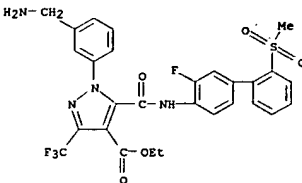
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L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 209958-22-5 CAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 1-[3-(aminomethyl)phenyl]-5-[[[3-fluoro-2'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-(trifluoromethyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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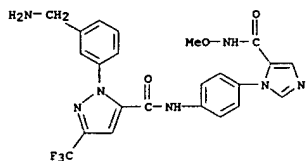
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CM 2

CRN 76-05-1
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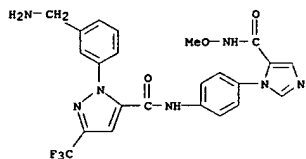
L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[5-(methoxyamino)carbonyl]-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209958-29-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-[5-(methoxyamino)carbonyl]-1H-imidazol-1-yl]phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209958-28-1
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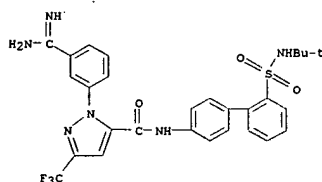
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L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

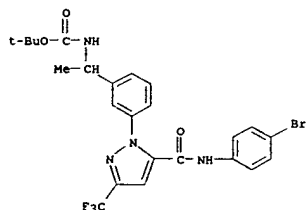


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IT 209960-02-1P 209960-07-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of nitrogen-containing heteroaroms. as factor Xa inhibitors)

RN 209960-02-1 CAPLUS
 CN Carbamic acid, [1-[3-[5-[[[4-bromophenyl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

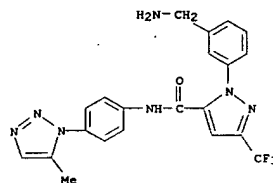


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10519356a.trn

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

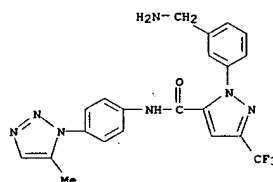
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RN 209958-31-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(5-methyl-1H-1,2,3-triazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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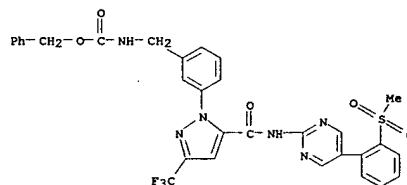
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CM 2

CRN 76-05-1
 CHF C2 H F3 O2

L9 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 pyrimidinyl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

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FULL ESTIMATED COST	199.57	423.85
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-28.08	-35.10

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PASSWORD:

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SESSION RESUMED IN FILE 'MEDLINE, CAPLUS' AT 09:03:35 ON 08 JAN 2007
FILE 'MEDLINE' ENTERED AT 09:03:35 ON 08 JAN 2007
FILE 'CAPLUS' ENTERED AT 09:03:35 ON 08 JAN 2007
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	ENTRY	SESSION
FULL ESTIMATED COST	199.57	423.85
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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CA SUBSCRIBER PRICE	-28.08	-35.10

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CA SUBSCRIBER PRICE	-28.08	-35.10

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L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
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 DOCUMENT NUMBER: 140:77148
 ENTRY DATE: Entered STN: 11 Jan 2004
 TITLE: Preparation of N-[4-(thioxoheterocyclyl)phenyl]-2-phenyl-2H-pyrazole-3-carboxamides and corresponding imino-heterocyclyl derivatives as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis
 INVENTOR(S): Cezanne, Bertram; Dorsch, Dieter; Mederski, Werner; Tsaklaidis, Christos; Gleitz, Johannes; Barnes, Christopher
 PATENT ASSIGNEE(S): Merck Patent GmbH, Germany
 SOURCE: PCT Int. Appl., 82 pp.
 DOCUMENT TYPE: CODEN: PIXXD2
 LANGUAGE: German
 INT. PATENT CLASSIF.:
 MAIN: A61K031-4155
 SECONDARY: A61K031-4178; A61K031-433; A61K031-42; C07D403-12; C07D417-12; C07D413-14; C07D403-14
 CLASSIFICATION: 28-B (Heterocyclic Compounds (More Than One Hetero Atom))
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION: Section cross-reference(s): 1, 63

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WO 2004002477	A1	20040108	WO 2003-EP5898	20030605
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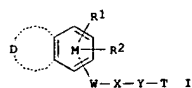
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L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 WO 2003-EP5898 W 20030605

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L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
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 C063/NA14; C063/ZA08; C063/ZA39; C063/ZA40;
 C063/ZA54; C063/ZA54; C063/ZB11; C063/ZB26;
 C063/ZC20
 EP 1679073 IPCI A61K031-4155 [I, A]; A61K031-4178 [I, A];
 A61K031-4164 [I, C*]; A61K031-433 [I, A]; A61K031-42 [I, A];
 C07D403-12 [I, A]; C07D417-12 [I, A]; C07D417-00
 [I, C*]; C07D413-14 [I, A]; C07D413-00 [I, C*];
 C07D403-14 [I, A]; C07D403-00 [I, C*];
 C07D403-12 [I, A]; C07D403/14; C07D413/14; C07D417/12
 C07D413-02 [ICM, 7]; C07D413-00 [ICM, 7, C*];
 A61K031-4709 [ICM, 7]; A61K031-4245 [ICM, 7];
 A61K031-423 [ICM, 7]
 IPCR A61K031-4155 [I, C*]; A61K031-4155 [I, A];
 A61K031-4164 [I, C*]; A61K031-4178 [I, A]; A61K031-42
 [I, C*]; A61K031-42 [I, A]; A61K031-433 [I, C*];
 A61K031-433 [I, A]; A61P0007-00 [I, C*]; A61P0007-02
 [I, A]; A61P0009-00 [I, C*]; A61P0009-08 [I, A];
 A61P0009-10 [I, A]; A61P0025-00 [I, C*]; A61P0025-06
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 NCL 514/310.000; 514/364.000; 514/375.000; 546/146.000;
 548/131.000; 548/215.000
 ECLA A61K031/4155; A61K031/4178; A61K031/42; A61K031/433;
 C07D403/12+231+207; C07D403/12+233+231;
 C07D413/14+261+231+207; C07D413/14+261+231+231;
 C07D417/12+285B+231
 MARPAT 140:77148

OTHER SOURCE(S):
 GRAPHIC IMAGE:



ABSTRACT:
 Title compds. [I: D = (N-, O-, S-interrupted) (substituted) C3-4 alkylene; M = Ph, aromatic heterocyclyl; R1, R2 = H, halo, (branched) (interrupted) (substituted) alkyl, NO2, cyano, OR3, N(R3)2, CO2R3, CON(R3)2, C(S)(R3)2, etc.; R3 = H, (branched) (interrupted) (substituted) alkyl, etc.; W = (substituted) (bicyclic aromatic (hetero) cyclyl; X = CONR3, CONR3(R4)2, C(R4)2NR3, etc.; R4 = H, (branched) (interrupted) (substituted) alkyl; Y =

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)
alkylene, cycloalkylene, heterodiy, arylidyl; T = (substituted) (bi)cyclic
arom. heterocyclyl], were prepd. Thus, 333 mg (3-[5-(4-[2-iminopyrrolidin-1-
yl]phenyl)carbamoyl]-3-trifluoromethylpyrazol-5-yl)benzyl)carbamoyl acid tert-Bu
ester (prepn. given) in EtOH was treated with HCl in ether to give 289 mg
N-[4-(2-iminopyrrolidin-1-yl)phenyl]-1-(3-aminomethylphenyl)-3-
(trifluoromethyl)-1H-pyrazole-5-carboxamide. The latter gave affinity to the
receptor Xa with IC50 = 9.6-10-9 M and to the receptor VIIa with IC50 =
2.3-10-8 M.

SUPPL. TERM: iminopyrrolidinylphenylphenylpyrazolecarboxamide prepn
coagulation factor Xa inhibitor; phenylpyrazolecarboxamide
iminopyrrolidinylphenyl prepn coagulation factor VIIa
inhibitor

INDEX TERM: Heart, disease
(angina pectoris, treatment; preparation of
(thiooxoheterocyclylphenyl) (phenylpyrazole)carboxamides
and corresponding imino-heterocyclyl derivs. as
inhibitors of the coagulation factors Xa and/or VIIa for
treating thrombosis)

INDEX TERM: Brain, disease
(cerebrovascular, treatment; preparation of
(thiooxoheterocyclylphenyl) (phenylpyrazole)carboxamides
and corresponding imino-heterocyclyl derivs. as
inhibitors of the coagulation factors Xa and/or VIIa for
treating thrombosis)

INDEX TERM: Artery, disease
(coronary, restenosis, treatment; preparation of
(thiooxoheterocyclylphenyl) (phenylpyrazole)carboxamides
and corresponding imino-heterocyclyl derivs. as
inhibitors of the coagulation factors Xa and/or VIIa for
treating thrombosis)

INDEX TERM: Heart, disease
(infarction, treatment; preparation of
(thiooxoheterocyclylphenyl) (phenylpyrazole)carboxamides
and corresponding imino-heterocyclyl derivs. as
inhibitors of the coagulation factors Xa and/or VIIa for
treating thrombosis)

INDEX TERM: Artery, disease
(intermittent claudication, treatment; preparation of
(thiooxoheterocyclylphenyl) (phenylpyrazole)carboxamides
and corresponding imino-heterocyclyl derivs. as
inhibitors of the coagulation factors Xa and/or VIIa for
treating thrombosis)

INDEX TERM: Neoplasm
(metastasis, treatment; preparation of
(thiooxoheterocyclylphenyl) (phenylpyrazole)carboxamides
and corresponding imino-heterocyclyl derivs. as
inhibitors of the coagulation factors Xa and/or VIIa for
treating thrombosis)

INDEX TERM: Headache
(migraine, treatment; preparation of
(thiooxoheterocyclylphenyl) (phenylpyrazole)carboxamides
and corresponding imino-heterocyclyl derivs. as
inhibitors of the coagulation factors Xa and/or VIIa for
treating thrombosis)

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)
boxamides and corresponding imino-heterocyclyl derivs.
as
inhibitors of the coagulation factors Xa and/or VIIa for
treating thrombosis)

INDEX TERM: 612841-24-4P 612841-31-3P 612841-32-4P 612841-34-6P
640287-98-5P 640287-99-6P 640288-00-2P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)

(thiooxoheterocyclylphenyl) (phenylpyrazole)car
boxamides and corresponding imino-heterocyclyl derivs.
as
inhibitors of the coagulation factors Xa and/or VIIa for
treating thrombosis)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD.

REFERENCE(S): (1) Du Pont Merck Pharma; WO 9828269 A 1998 CAPLUS
(2) Du Pont Merck Pharma; WO 9857937 A 1998 CAPLUS
(3) Du Pont Merck Pharma; WO 9857951 A 1998 CAPLUS

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)
INDEX TERM: Anti-inflammatory agents
Antiarteriosclerotics
Anticoagulants
Antimigraine agents
Antitumor agents
Human
(preparation of
(thiooxoheterocyclylphenyl) (phenylpyrazole)car
boxamides and corresponding imino-heterocyclyl derivs.
as
inhibitors of the coagulation factors Xa and/or VIIa for
treating thrombosis)

INDEX TERM: Arteriosclerosis
Inflammation
Neoplasm
Thrombosis
(treatment; preparation of
(thiooxoheterocyclylphenyl) (phenylp
yrazole)carboxamides and corresponding
imino-heterocyclyl
derivs. as inhibitors of the coagulation factors Xa
and/or VIIa for treating thrombosis)

INDEX TERM: 9002-05-5, Coagulation factor Xa 65312-43-8, Coagulation
factor VIIa
ROLE: BSU (Biological study, unclassified); BIOL
(Biological
study)
(inhibitors; preparation of
(thiooxoheterocyclylphenyl) (phenyl
pyrazole)carboxamides and corresponding
imino-heterocyclyl derivs. as inhibitors of the
coagulation factors Xa and/or VIIa for treating
thrombosis)

INDEX TERM: 640287-97-4P 640288-03-5P 640288-05-7P 640288-06-8P
640288-07-9P 640288-11-5P 640288-12-6P 640288-13-7P
640288-14-8P 640288-15-9P 640288-16-0P 640288-17-1P
640288-18-2P 640288-19-3P 640288-20-6P 640288-21-7P
640288-22-8P 640288-23-9P 640288-24-0P 640288-25-1P
640288-26-2P 640288-27-3P 640288-28-4P 640288-29-5P
640288-30-8P
ROLE: PAC (Pharmacological activity); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological
study); PREP (Preparation); USES (Uses)

(preparation of
(thiooxoheterocyclylphenyl) (phenylpyrazole)car
boxamides and corresponding imino-heterocyclyl derivs.
as
inhibitors of the coagulation factors Xa and/or VIIa for
treating thrombosis)

INDEX TERM: 209917-93-1 438056-68-9 443999-53-9 625101-83-9
625101-85-1 640288-01-3 640288-02-4 640288-04-6
640288-08-0 640288-09-1 640288-10-4
ROLE: RCT (Reactant); RACT (Reactant or reagent)

(preparation of
(thiooxoheterocyclylphenyl) (phenylpyrazole)car

Page 114

=> d hitstr

10519356a.trn

=> d str
'STR' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS ----- GI and AB
ALL ----- BIB, AB, IND, RE
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data and PI table (default)
CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
CLASS ----- IPC, NCL, ECLA, FTERM
DALL ----- ALL, delimited (end of each field identified)
DMAX ----- MAX, delimited for post-processing
FAM ----- AN, PI and PRAI in table, plus Patent Family data
FBIB ----- AN, BIB, plus Patent FAM
IND ----- Indexing data
IPC ----- International Patent Classifications
MAX ----- ALL, plus Patent FAM, RE
PATS ----- PI, SO
SAM ----- CC, SX, TI, ST, IT
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
SCAN must be entered on the same line as the DISPLAY,
e.g., D SCAN or DISPLAY SCAN)
STD ----- BIB, CLASS

IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IMAX ----- MAX, indented with text labels
ISTD ----- STD, indented with text labels

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

HIT ----- Fields containing hit terms
HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
containing hit terms
HITRN ----- HIT RN and its text modification
HITSTR ----- HIT RN, its text modification, its CA index name, and
its structure diagram
HITSEQ ----- HIT RN, its text modification, its CA index name, its
structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
structure diagram, plus NTE and SEQ fields
KWIC ----- Hit term plus 20 words on either side
OCC ----- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the

information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.

ENTER DISPLAY FORMAT (BIB):hitrn

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
FULL ESTIMATED COST	ENTRY	SESSION
	8.94	432.79
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
	-0.78	-35.88

FILE 'REGISTRY' ENTERED AT 09:08:28 ON 08 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 7 JAN 2007 HIGHEST RN 916885-50-2
DICTIONARY FILE UPDATES: 7 JAN 2007 HIGHEST RN 916885-50-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> S 640287-97-4/RN

L11 1 640287-97-4/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D L11 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):n

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=>

=> d his

(FILE 'HOME' ENTERED AT 07:49:52 ON 08 JAN 2007)

FILE 'REGISTRY' ENTERED AT 07:50:03 ON 08 JAN 2007

L1 STRUCTURE UPLOADED
L2 50 L1

FILE 'CAPLUS' ENTERED AT 07:50:41 ON 08 JAN 2007

L3 28 L2

FILE 'REGISTRY' ENTERED AT 07:51:35 ON 08 JAN 2007

L4 STRUCTURE UPLOADED
L5 50 L4
L6 STRUCTURE UPLOADED
L7 22 L6
L8 426 L6 FULL

FILE 'MEDLINE, CAPLUS' ENTERED AT 07:56:10 ON 08 JAN 2007

L9 36 L8

FILE 'CAPLUS' ENTERED AT 09:03:48 ON 08 JAN 2007

E US 2004-519356/AP,PRN 25
L10 1 S E3

FILE 'REGISTRY' ENTERED AT 09:08:28 ON 08 JAN 2007

L11 1 S 640287-97-4/RN
SET NOTICE 1 DISPLAY
SET NOTICE LOGIN DISPLAY

=> d hitstr

'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information

BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

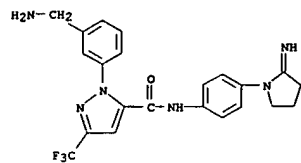
The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):sam

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
 IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)-, dihydrochloride (9CI)
 MF C22 H21 F3 N6 O . 2 Cl H



● 2 HCl

=> 640287-97-4P 640288-03-5P 640288-05-7P 640288-06-8P 640288-11-5P
 640288-12-6P 640288-13-7P 640288-14-8P 640288-15-9P
 640288-16-0P 640288-17-1P

PROXIMITY OPERATOR LEVEL NOT CONSISTENT WITH
 FIELD CODE - 'AND' OPERATOR ASSUMED '0287-97-4P(W) 640288-03-'
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 FIELD CODE - 'AND' OPERATOR ASSUMED '0288-05-7P(W) 640288-06-'
 PROXIMITY OPERATOR LEVEL NOT CONSISTENT WITH
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 FIELD CODE - 'AND' OPERATOR ASSUMED '0288-15-9P(W) 640288-16-'
 PROXIMITY OPERATOR LEVEL NOT CONSISTENT WITH
 FIELD CODE - 'AND' OPERATOR ASSUMED '0288-16-0P(W) 640288-17-'

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 (640288-17-1P/RN)

L12 0 640287-97-4P 640288-03-5P 640288-05-7P 640288-06-8P 64028
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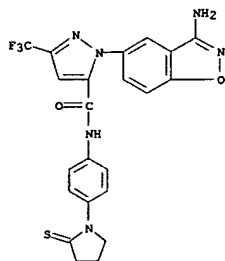
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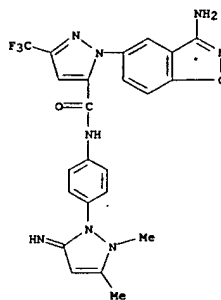
=> d sam 1-12

L13 ANSWER 1 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C22 H17 F3 N6 O2 S



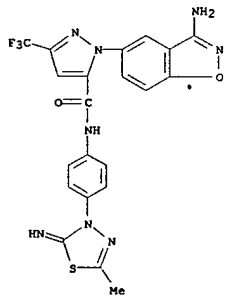
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 2 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2,5-dihydro-5-imino-2,3-dimethyl-1H-pyrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C23 H19 F3 N8 O2



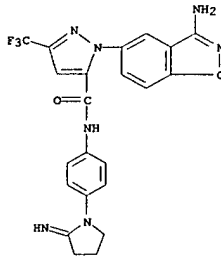
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 3 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-imino-5-methyl-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C21 H15 F3 N8 O2 S



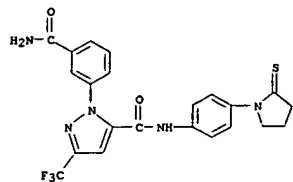
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 4 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C22 H18 F3 N7 O2



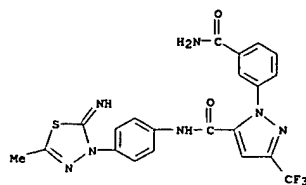
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 5 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C22 H18 F3 N5 O2 S



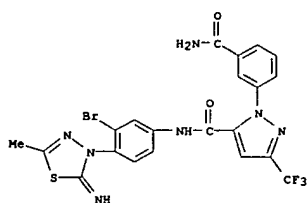
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 6 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-imino-5-methyl-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI)
MF C21 H16 F3 N7 O2 S



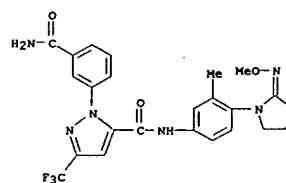
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 7 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
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MF C21 H15 Br F3 N7 O2 S



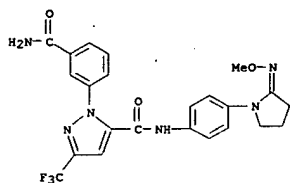
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 8 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-[2-(methoxyimino)-1-pyrrolidinyl]-3-methylphenyl]-3-(trifluoromethyl)- (9CI)
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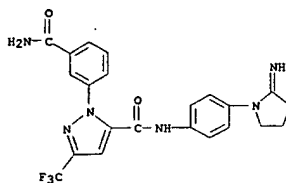
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 9 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
 IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-[2-(methoxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI)
 MF C23 H21 F3 N6 O3



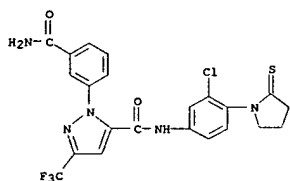
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 10 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
 IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI)
 MF C22 H19 F3 N6 O2



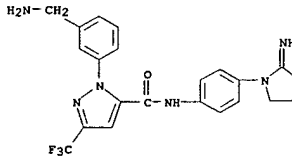
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 11 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
 IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[3-chloro-4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI)
 MF C22 H17 Cl F3 N5 O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 12 OF 12 REGISTRY COPYRIGHT 2007 ACS on STN
 IN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)-, dihydrochloride (9CI)
 MF C22 H21 F3 N6 O . 2 Cl H



● 2 HCl

=> log h

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

16.66

449.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-35.88

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 09:13:37 ON 08 JAN 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAJRK1626

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *

SESSION RESUMED IN FILE 'REGISTRY' AT 10:03:28 ON 08 JAN 2007

FILE 'REGISTRY' ENTERED AT 10:03:28 ON 08 JAN 2007

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

16.66

449.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

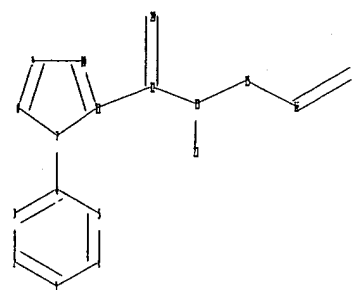
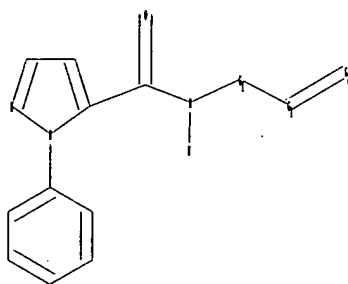
CA SUBSCRIBER PRICE

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ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
4-7 11-12 12-13 12-20 13-15 13-21 15-16 16-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11
exact/norm bonds :
4-7 7-8 7-11 8-9 9-10 10-11 12-13 12-20 13-15 15-16 16-19
exact bonds :
11-12 13-21
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
  
```

G1:Cb,Cy,Hy

G2:S,N

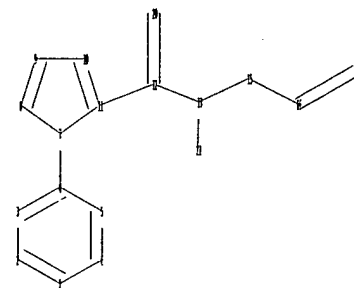
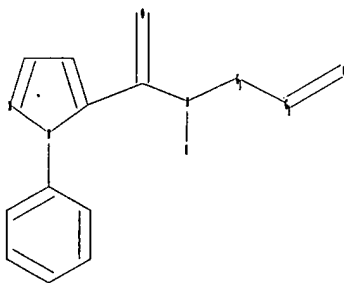
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 15:CLASS 16:CLASS 19:CLASS 20:CLASS 21:CLASS

L14 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\10519356\Struc 8.str



chain nodes :

12 13 15 16 19 20 21

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

4-7 11-12 12-13 12-20 13-15 13-21 15-16 16-19

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11

exact/norm bonds :

4-7 7-8 7-11 8-9 9-10 10-11 12-13 12-20 13-15 15-16 16-19

10519356a.trn

exact bonds :

11-12 13-21

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:Cb,Cy,Hy

G2:S,N

G3:Cb,Cy,Hy,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

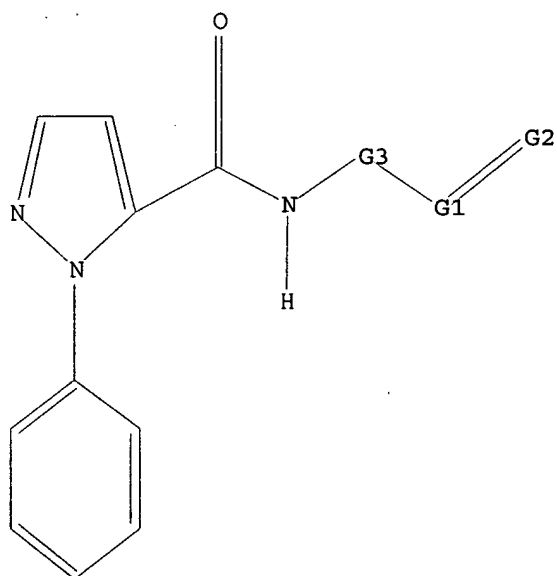
11:Atom 12:CLASS 13:CLASS 15:CLASS 16:CLASS 19:CLASS 20:CLASS 21:CLASS

L15 STRUCTURE UPLOADED

=> d

L15 HAS NO ANSWERS

L15 STR



G1 Cb,Cy,Hy

G2 S,N

G3 Cb,Cy,Hy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> l15

SAMPLE SEARCH INITIATED 10:05:17 FILE 'REGISTRY'

10519356a.trn

SAMPLE SCREEN SEARCH COMPLETED - 302 TO ITERATE

100.0% PROCESSED 302 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 4998 TO 7082
PROJECTED ANSWERS: 1 TO 80

L16 1 SEA SSS SAM L15

=> l15 full
FULL SEARCH INITIATED 10:05:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 5859 TO ITERATE

100.0% PROCESSED 5859 ITERATIONS 30 ANSWERS
SEARCH TIME: 00.00.01

L17 30 SEA SSS FUL L15

=> file medline caplus		
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	ENTRY	SESSION
FULL ESTIMATED COST	189.66	622.45
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-35.88

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FILE 'CAPLUS' ENTERED AT 10:05:33 ON 08 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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=> l17
L18 5 L17

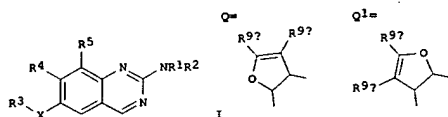
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L18 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 2006:1176145 CAPLUS
 DOCUMENT NUMBER: 145:489261
 TITLE: Preparation of 2-aminoquinazoline derivatives as p38 mitogen-activated protein kinase inhibitors
 INVENTOR(S): Kishikawa, Kuniyuki; Imase, Hidetomo; Kashima, Hajime;
 Mori, Kiyotoshi; Ikemura, Toshihide; Nakasato, Yoshisuke; Tomuro, Misato
 PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 265pp.
 CODEN: PIXMD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006118256	A1	20061109	WO 2006-JP309000	20060428
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CP, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, GU, HK, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, GM, HR, KE, MG, ML, MR, NE, NG, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

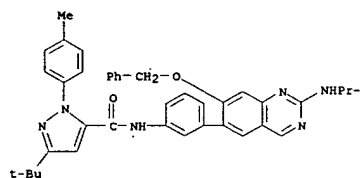
PRIORITY APPLN. INFO.: JP 2005-130704 A 20050428

OTHER SOURCE(S): MARPAT 145:489261
 GI

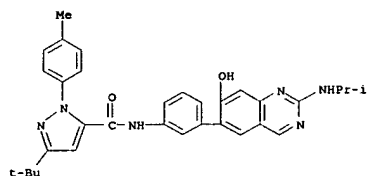


AB 2-Aminoquinazoline and 2-aminofuro[2,3-h]quinazoline derivs. represented by the general formula (I) or pharmacol. acceptable salts thereof [wherein
 R1, R2 = H, each (un)substituted lower alkyl, lower alkenyl, alkynyl, cycloalkyl, cycloalkenyl, lower alkanoyl, cycloalkylcarbonyl, aryl, heterocyclyl, CONH2; X = a bond, (un)substituted CH2; when X = a bond, R3 = (un)substituted aryl or aromatic heterocyclyl; when X = (un)substituted

L18 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)
 CH2, R3 = each (un)substituted lower alkoxy, aryl, arom. heterocyclyl, or CONH2; R4 = H, halo, HO, each (un)substituted lower alkyl, lower alkenyl, lower alkynyl, lower alkoxy, lower alkanoyloxy, aryl, aryloxy, or heterocyclyl; R5 = H, halo, HO, each (un)substituted lower alkyl, lower alkenyl, lower alkoxy, aryl, heterocyclyl, or CONH2; or R4 and R5 together with the adjacent carbon atoms represent Q or Q1; R9a, R9b = H, halo, HO, each (un)substituted lower alkyl, lower alkenyl, lower alkoxy, lower alkoxy carbonyl, aryl, heterocyclyl, or CONH2 are prep. These compds. are useful as p38 mitogen-activated protein (P38MAP) kinase inhibitors for the prevention and/or treatment of diseases related to the function of P38MAP kinase, e.g. inflammations, chronic articular rheumatism, osteoarthritis, arthritis, osteoporosis, autoimmune diseases, blood poisoning, cachexia, cerebral infarction, Alzheimer's disease, asthma, a chronic pneumonia, chronic obstructive pulmonary disease (COPD), thrombosis, glomerulonephritis, diabetes, host vs. graft rejection, inflammatory bowel disease, Crohn's disease, ulcerative colitis, multiple sclerosis, tumor proliferation and metastasis, multiple myeloma. Thus, 1.20 g 6-bromo-2-isopropylamino-7-methoxyquinazoline was dissolved in 20 mL dioxane and 20 mL H2O, treated with 0.900 g 2-chlorophenylboric acid, 1.03 g Na2CO3, and 197 mg [1,1'-bis(diphenylphosphino)ferrocene]dichloro-palladium, and the resulting mixt. was heated under refluxing for 2 h to give, after workup and silica gel chromatog., 66% 6-(2-chlorophenyl)-2-isopropylamino-7-methoxyquinazoline (II). II at 1 µM inhibited 250% human P38MAP.
 IT 914396-51-3P, 7-Benzyl-6-[3-[[[5-tert-butyl-2-(4-methylphenyl)-2H-pyrazol-3-yl]carbonyl]amino]phenyl]-2-(isopropylamino)quinazoline 914396-52-4P, 6-[3-[[[5-tert-butyl-2-(4-methylphenyl)-2H-pyrazol-3-yl]carbonyl]amino]phenyl]-7-hydroxy-2-(isopropylamino)quinazoline
 RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of 2-aminoquinazoline derivs. as p38 mitogen-activated protein kinase inhibitors)
 RN 914396-51-3 CAPLUS
 CN INDEX NAME NOT YET ASSIGNED

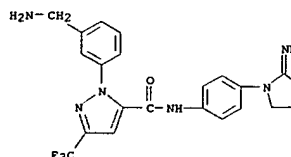


L18 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)
 RN 914396-52-4 CAPLUS
 CN INDEX NAME NOT YET ASSIGNED



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L18 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 2006:1061760 CAPLUS
 TITLE: Design and Evaluation of a Novel Class-Directed 2D Fingerprint to Search for Structurally Diverse Active Compounds
 AUTHOR(S): Eckert, Hanna; Bajorath, Juergen
 CORPORATE SOURCE: Department of Life Science Informatics, B-IT, Rheinische Friedrich-Wilhelms-Universitaet, Bonn, D-53113, Germany
 SOURCE: Journal of Chemical Information and Modeling (2006), 46(6), 2515-2526
 CODEN: JCISDH; ISSN: 1549-9596
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Recent attempts to increase similarity search performance using mol. fingerprints have mostly focused on the evaluation of alternative similarity metrics or scoring schemes, rather than the development of new types of fingerprints. Here, the authors introduce a novel 2D fingerprint design (property descriptor value range-derived fingerprint or PDR-FP) that involves activity-oriented selection of property descriptors and the transformation of descriptor value ranges into a binary format such that each fingerprint bit position represents a specific value interval. The design is tailored toward multiple-template similarity searching and permits training on specific activity classes. In search calcs. on 15 compound classes of increasing structural diversity, the PDR fingerprint performed better than other state-of-the-art 2D fingerprints. Among the structurally diverse classes were six compound sets with peptide character, which represent a notoriously difficult chemotype for 2D similarity searching. In these cases, PDR-FP produced promising results, whereas other fingerprint methods mostly failed. PDR-FP is specifically designed for search calcs. on structurally diverse compds., and these calcs. are not influenced by mol. size effects, which represent a general problem for similarity searching using bit string representations.
 IT 774536-86-6
 RI: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PRP (Properties); USES (Uses)
 (design and evaluation of a class-directed 2D fingerprint to search for structurally diverse active compds.)
 RN 774536-86-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-(4-(2-imino-1-pyrrolidinyl)phenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



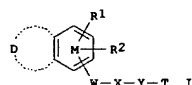
L18 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
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L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:20490 CAPLUS
 DOCUMENT NUMBER: 140:77148
 TITLE: Preparation of N-[4-(thioxoheterocyclyl)phenyl]-2-phenyl-2H-pyrazole-3-carboxamides and corresponding imino-heterocyclyl derivatives as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis
 INVENTOR(S): Cezanne, Bertram; Dorsch, Dieter; Mederski, Werner; Tsaklakis, Christos; Gleitz, Johannes; Barnes, Christopher
 PATENT ASSIGNEE(S): Merck Patent GmbH, Germany
 SOURCE: PCT Int. Appl., 82 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004002477	A1	20040108	WO 2003-EP5898	20030605
WO 2004002477	A8	20040415		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10229070	A1	20040115	DE 2002-10229070	20020628
CA 2491271	A1	20040108	CA 2003-2491271	20030605
AU 2003238475	A1	20040119	AU 2003-238475	20030605
EP 1517685	A1	20050330	EP 2003-732540	20030605
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JP 2005535630	T	20051124	JP 2004-516575	20030605
EP 1679073	A1	20060712	EP 2006-157	20030605
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US 2005203127	A1	20050915	US 2004-519356	20041228
PRIORITY APPLN. INFO.: DE 2002-10229070 A 20020628				
EP 2003-732540 A3 20030605				
WO 2003-EP5898 W 20030605				

OTHER SOURCE(S): MARPAT 140:77148
 GI

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB Title compds. [I; D = (N-, O-, S-interrupted) (substituted) C3-4 alkylene:
 M = Ph, aromatic heterocyclyl; R1, R2 = H, halo, (branched) (interrupted) (substituted) alkyl, NO2, cyano, OR3, N(R3)2, CO2R3, CON(R3)2, C(S)N(R3)2, etc.; R3 = H, (branched) (interrupted) (substituted) alkyl, etc.; W = (substituted) (bi)cyclic aromatic (heterocyclyl); X = CONR3, CONR3C(R4)2, C(R4)2NR3, etc.; R4 = H, (branched) (interrupted) (substituted) alkyl; Y = alkylene, cycloalkylene, heterodiy, aryldiy; T = (substituted) (bi)cyclic aromatic heterocyclyl, were prepared Thus.
 333 mg

(3-[5-(4-[2-iminopyrrolidin-1-yl]phenyl)carbamoyl]-3-trifluoromethylpyrazol-1-yl)benzyl)carbamoyl acid tert-Bu ester (preparation given) in EtOH was treated

with HCl in ether to give 289 mg
 N-[4-(2-iminopyrrolidin-1-yl)phenyl]-1-(3-aminomethylphenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide. The latter gave affinity to the receptor Xa with IC50 = 9.6·10⁻⁹ M and to the receptor VIIa with IC50 = 2.3·10⁻⁸ M.

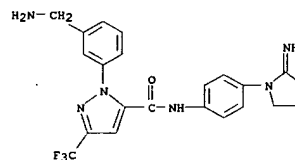
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 640288-27-3P 640288-28-4P 640288-30-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (thioxoheterocyclyl)phenyl) (phenyl)pyrazole)carboxamides and corresponding imino-heterocyclyl derivs. as inhibitors of the coagulation factors Xa and/or VIIa for treating thrombosis)

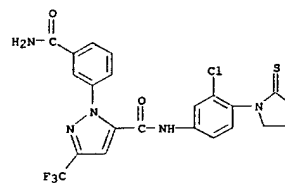
RN 640287-97-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)-, dihydrochloride (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

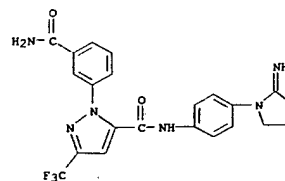


● 2 HCl

RN 640288-03-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[3-chloro-4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

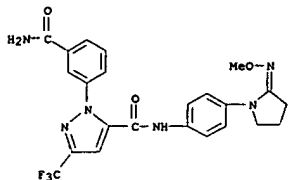


RN 640288-05-7 CAPLUS
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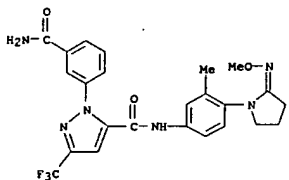


RN 640288-06-8 CAPLUS

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-methoxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

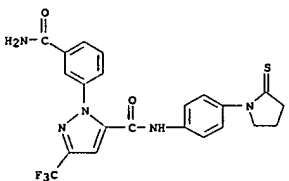


RN 640288-07-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-methoxyimino)-1-pyrrolidinyl]-3-methylphenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

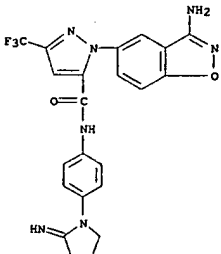


RN 640288-11-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[3-bromo-4-(2-imino-5-methyl-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

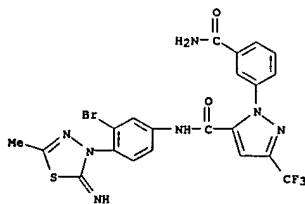


RN 640288-14-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-imino-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

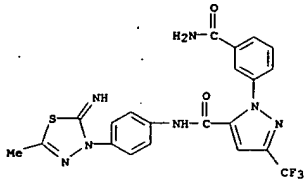


RN 640288-15-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-imino-5-methyl-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

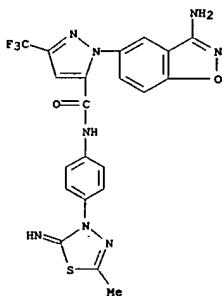


RN 640288-12-6 CAPLUS
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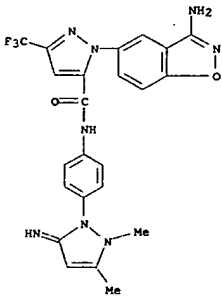


RN 640288-13-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

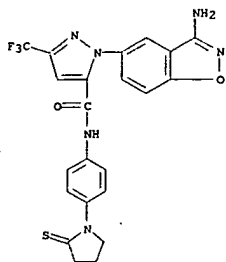


RN 640288-16-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2,5-dihydro-5-imino-2,3-dimethyl-1H-pyrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

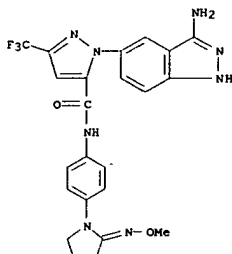


RN 640288-17-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

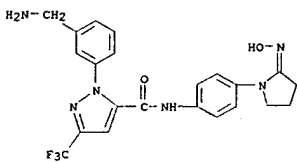


RN 640288-18-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-amino-1H-indazol-5-yl]-N-[4-(2-methoxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

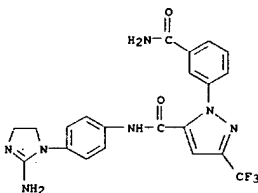


RN 640288-19-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-amino-1H-indazol-5-yl]-N-[4-(2-thioxo-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

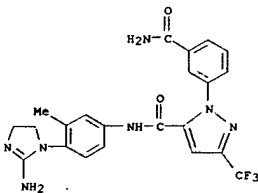
L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 640288-22-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-amino-4,5-dihydro-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



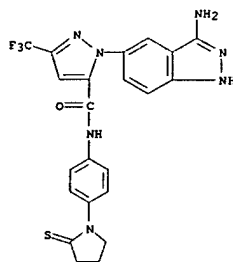
RN 640288-23-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-amino-4,5-dihydro-1H-imidazol-1-yl)-3-methylphenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



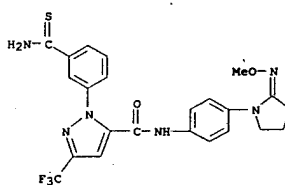
RN 640288-24-0 CAPLUS

10519356a.trn

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



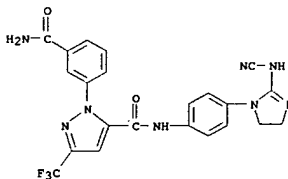
RN 640288-20-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminothioxomethyl)phenyl]-N-[4-(2-methoxyimino)-1-pyrrolidinyl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



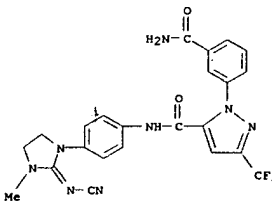
RN 640288-21-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2-(hydroxyimino)-1-pyrrolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-(cyanoimino)-4,5-dihydro-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

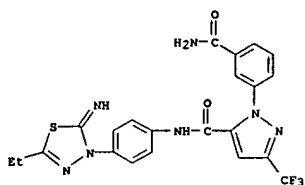


RN 640288-25-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(2-(cyanoimino)-3-methyl-1-imidazolidinyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

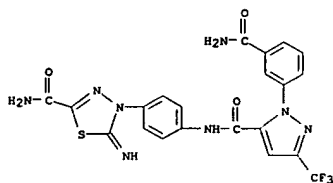


RN 640288-26-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(5-ethyl-2-imino-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

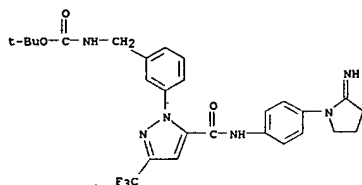


RN 640288-27-3 CAPLUS
 CN 1,3,4-Thiadiazole-2-carboxamide, 4-[[4-[[[1-[3-(aminocarbonyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-4,5-dihydro-5-imino- (9CI) (CA INDEX NAME)



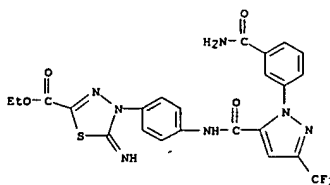
RN 640288-28-4 CAPLUS
 CN 1,3,4-Thiadiazole-2-carboxylic acid, 4-[[4-[[[1-[3-(aminocarbonyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-4,5-dihydro-5-imino-, ethyl ester (9CI) (CA INDEX NAME)

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

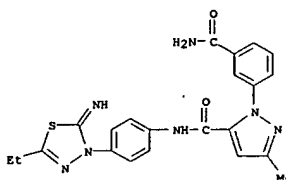


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 640288-30-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminocarbonyl)phenyl]-N-[4-(5-ethyl-2-imino-1,3,4-thiadiazol-3(2H)-yl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)



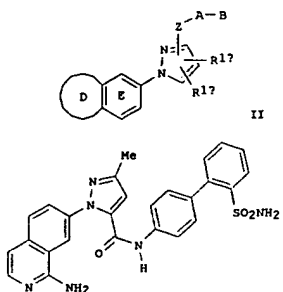
IT 640288-00-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (Preparation of
 (thioxoheterocyclylphenyl)(phenylpyrazole)carboxamides and
 corresponding imino-heterocyclyl derivs. as inhibitors of the
 coagulation factors Xa and/or VIIa for treating thrombosis)
 RN 640288-00-2 CAPLUS
 CN Carbamic acid,
 [[3-[5-[[[4-(2-imino-1-pyrrolidinyl)phenyl]amino]carbonyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methyl]-, 1,1-dimethylethyl
 ester (9CI) (CA INDEX NAME)

L18 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:39605 CAPLUS
 DOCUMENT NUMBER: 136:102380
 TITLE: Preparation of novel guanidine mimics as factor Xa inhibitors
 INVENTOR(S): Lam, Patrick Y.; Clark, Charles G.; Dominguez, Celia; Fevig, John M.; Han, Qi; Li, Renhua; Pinto, Donald J. P.; Pruitt, James R.; Quan, Mimi L.
 PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA
 SOURCE: U.S., 117 pp.
 CODEN: USXGAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

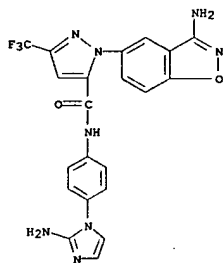
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6339099	B1	20020115	US 1998-99358	19980618
US 2002025963	A1	20020228	US 2001-924381	20010808
US 6906070	B2	20050614		
US 2003069258	A1	20030410	US 2002-98994	20020313
US 6958356	B2	20051025		
US 2004063772	A1	20040401	US 2003-602214	20030624
US 6965036	B2	20051115		
US 2006040973	A1	20060223	US 2005-197978	20050805
			US 1997-50265P	P 19970620
			US 1998-99358	A3 19980618
			US 2001-924381	B1 20010808
			US 2002-98994	A1 20020313

OTHER SOURCE(S): MARPAT 136:102380
 GI



AB The title compds. [I; ring D = 5-membered aromatic system containing
from 1-2
heteroatoms selected from N, O, S; ring D is substituted with 0-2 R
groups; ring E contains 0-2 N atom and is substituted by 0-1 R groups; R
= Cl, F, Br, I, OH, alkoxy, amino(alkyl), (alkyl)amino; Z = bond, alkylene,
(CH₂)rO(CH₂)r, (CH₂)rNR3(CH₂)r, (CH₂)rC(O)(CH₂)r, (CH₂)rO(CH₂)r,
(CH₂)rOC(O)(CH₂)r, (CH₂)rC(O)(CH₂)rNR3(CH₂)r, etc. provided that Z does not
form
a N-N, N-O, N-S, NCH₂N, NCH₂O, or NCH₂S bond with ring M or group A;
R1a-1b = H, alk(en)yl, aminoalkyl, alkyl, alternatively, R1a-1b, when
attached to adjacent carbon atoms, together with the atoms to which they
are attached form a 5-8 membered (un)saturated ring (un)substituted and
which
contains from 0-2 heteroatoms selected from the group consisting of N, O,
and S; alternatively, when Z is C(O)NH and R1a is attached to a ring
carbon adjacent to Z, then R1a is a C(O) which replaces the amide
hydrogen
of Z to form a cyclic imide; R3 = H, alkyl, phenyl; A = (un)substituted
carbocyclic, 5-10 membered heterocyclic system containing 1-4 heteroatoms
selected from N, O, S; B = H, X, X-Y; X = sulfonylalkyl, alkylsulfonyl,
sulfonamide, etc.; Y = alkylamino, provided that X-Y does not form a N-N,
O-N or S-N bond, carbocyclic group, 5-10 membered heterocyclic r = 0-3),
inhibitors of factor Xa which are useful in treating and preventing a
thromboembolic disorder, were prepared and formulated. Thus, a
multi-step
synthesis of the title compound II, starting with 7-aminoisoquinoline,
was
described. A number of compds. I were found to exhibit a Ki of ≤ 15
 μ M against factor Xa.
IT 218298-55-6P 218299-98-OP

L18 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

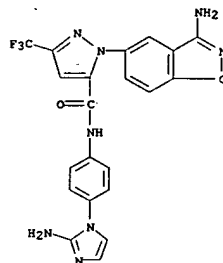
CRN 76-05-1

CMF C2 H F3 O2



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
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L18 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)
 LR: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (prepn. of novel guanine mimics as factor Xa inhibitors)
 RN 21829-55-6 CAPLUS
 CN 1R-Pyrazole-5-carboxamide,
 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-amino-
 1R-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (SCI) (CA INDEX NAME)



```

RN      218299-98-0  CAPLUS
CN      1H-Pyrazole-5-carboxamide,
1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-amino-
1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate)
(SC1)   (CA INDEX NAME)

CH      1

CRN     218298-55-6
CMF     C21 H15 F3 N8 O2

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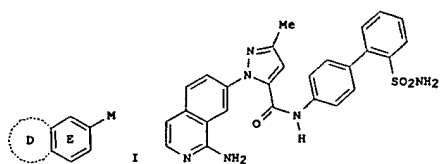
L18 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:9833 CAPLUS
DOCUMENT NUMBER: 130:66494
TITLE: Preparation of novel guanidine mimics as factor Xa inhibitors
INVENTOR(S): Lam, Patrick Y.; Clark, Charles G.; Dominguez, Celia; Fevig, John Matthew; Han, Qi; Li, Renhua; Pinto, Donald Joseph-Phillip; Pruitt, James Russell; Quan, Mimi Lifan
PATENT ASSIGNEE(S): The Du Pont Merck Pharmaceutical Company, USA
SOURCE: PCT Int. Appl., 268 pp.
CODING: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATEM NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9857951	A1	19981223	WO 1998-US12680	19980618
W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE	A	19991217	ZA 1998-5247	19980617
ZA 9805247	A1	19991223	ZA 1998-291442	19980618
CA 2291442	A1	19990124	AU 1998-79768	19980618
AU 9879768	B2	20010123		
AU 756755	A1	20000412	EP 1998-930361	19980618
EP 991638	B1	20050817		
EP 991638	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO			
BR 9810137	A	20000808	BR 1998-10137	19980618
EE 9900583	A	20000815	EE 1999-583	19980618
EE 4153	B1	20031015		
HU 200002686	A2	20020128	HU 2000-2686	19980618
JP 2002505668	T	20020219	JP 1999-504785	19980618
NZ 502370	A	20021025	NZ 1998-502370	19980618
AT 302198	T	20050915	AT 1998-930361	19980618
ES 2244064	T3	20051201	ES 1998-930361	19980618
RO 120543	B1	20060330	RO 1999-1317	19980618
TW 544453	B	20030801	TW 1998-87109910	19980819
NO 9905965	A	19991203	NO 1999-5965	19991203
NO 318359	B1	20050307		
MX 9911908	A	20000531	MX 1999-11908	19991216
LV 12496	B	20010128	LV 1999-178	19991216
LT 4705	B	20000925	LT 1999-147	19991217
PRIORITY APPLN. INFO.:			US 1997-878884	A 19970619
			WO 1998-US12680	W 19980618

OTHER SOURCE(S): MARPAT 130:66494
GI

L18 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



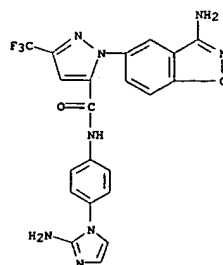
II

AB The title compds. [I: rings D-E represent guanidine mimics; ring D = CH2N:CH, CH2CH2N:CH, a 5-6 membered aromatic system containing 0-2 heteroatoms selected form the group N, O, and S; ring E is substituted with 0-2 R (substituents), provided that when ring D is unsubstituted, it contains at least one heteroatom; ring E contains 0-2 N atom and is substituted by 0-1 R; R = halo, OH, Cl-3 alkoxy, etc.; M = (un)substituted pyrazole, imidazole, tetrazole, etc.], inhibitors of factor Xa which are useful in treating and preventing a thromboembolic disorder, were prepared and formulated. Thus, a multi-step synthesis of the title compound II, starting with 7-aminoisoquinoline, was described. A number of compds. I were found to exhibit a Ki of ≤ 15 μ M against factor Xa.

IT 218298-55-6P 218299-98-0P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of novel guanidine mimics as factor Xa inhibitors)

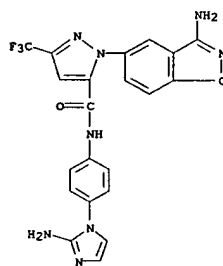
RN 218298-55-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-amino-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 218299-98-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-amino-1H-imidazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1
 CRN 218298-55-6
 CMF C21 H15 F3 N8 O2



L18 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 2
 CRN 76-05-1
 CMF C2 H F3 O2



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

28.75

651.20

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CAS SUBSCRIBER PRICE

-3.90

-39.78

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STRUCTURE FILE UPDATES: 7 JAN 2007 HIGHEST RN 916885-50-2

DICTIONARY FILE UPDATES: 7 JAN 2007 HIGHEST RN 916885-50-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

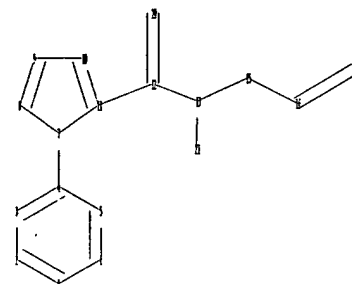
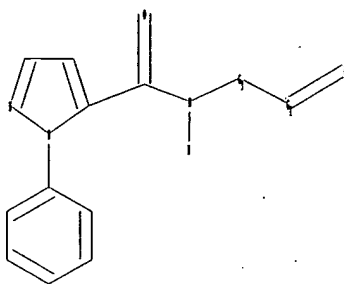
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

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chain nodes :
12 13 15 16 19 20 21
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
4-7 11-12 12-13 12-20 13-15 13-21 15-16 16-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11
exact/norm bonds :
4-7 7-8 7-11 8-9 9-10 10-11 12-13 12-20 13-15 15-16 16-19
exact bonds :
11-12 13-21
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

```

G1:Cb,Cy,Hy

G2:S,N,O

G3:Cb,Cy,Hy,Ak

Match level :

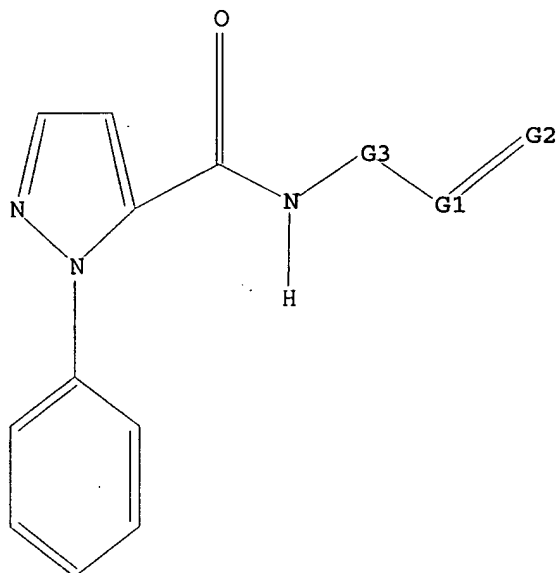
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11:Atom 12:CLASS 13:CLASS 15:CLASS 16:CLASS 19:CLASS 20:CLASS 21:CLASS

L19 STRUCTURE UPLOADED

=> d

L19 HAS NO ANSWERS

L19 STR



G1 Cb,Cy,Hy

G2 S,N,O

G3 Cb,Cy,Hy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> 119

SAMPLE SEARCH INITIATED 10:08:24 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 319 TO ITERATE

100.0% PROCESSED 319 ITERATIONS

5 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 5309 TO 7451

PROJECTED ANSWERS: 5 TO 234

L20 5 SEA SSS SAM L19

=> l19 full

FULL SEARCH INITIATED 10:08:28 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 6149 TO ITERATE

100.0% PROCESSED 6149 ITERATIONS
SEARCH TIME: 00.00.01

82 ANSWERS

L21 82 SEA SSS FUL L19

=> file medline caplus

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

172.10

823.30

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

ENTRY

TOTAL

SESSION

CA SUBSCRIBER PRICE

0.00

-39.78

FILE 'MEDLINE' ENTERED AT 10:08:36 ON 08 JAN 2007

FILE 'CAPLUS' ENTERED AT 10:08:36 ON 08 JAN 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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=> l21

L22 11 L21

=> l22 not l18

L23 6 L22 NOT L18

=> d ibib abs hitstr 1-6

L23 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2004:791919 CAPLUS

DOCUMENT NUMBER:

141:342889

TITLE:

SAR and factor IXa crystal structure of a dual inhibitor of factors IXa and Xa
Smallheer, Joanne M.; Alexander, Richard S.; Wang, Jianmin; Wang, Shuaige; Nakajima, Suanne; Rossi, Karen

AUTHOR(S):

Karen

Debra:

A.; Smallwood, Angela; Barbera, Frank; Burdick,

CORPORATE SOURCE:

Luetgten, Joseph M.; Knabb, Robert M.; Wexler, Ruth R.; Jadhav, Prabhakar K.
Bristol-Myers Squibb Company, Princeton, NJ,

SOURCE:

08543-5400, USA
Bioorganic & Medicinal Chemistry Letters (2004),

PUBLISHER:

14(21), 5263-5267

DOCUMENT TYPE:

CODEN: BMCLE8; ISSN: 0960-894X

LANGUAGE:

Elsevier B.V.

OTHER SOURCE(S):

Journal

CASREACT 141:342889

AB

Modifications to the P4 moiety and pyrazole C3 substituent of factor Xa inhibitor SN-429 provided several new compounds, which are 5-10 nM inhibitors of factor IXa. An x-ray crystal structure of one example complexed to factor IXa shows that these compounds adopt a similar binding mode to that previously observed with pyrazole inhibitors in the factor

Xa

active site both with regard to how the inhibitor binds and the position of Tyr99.

IT

848393-99-7P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(pyrazole compounds, preparation, crystal structure, and dual inhibition of factors IXa and Xa)

of

RN

848393-99-7 CAPLUS

CN

1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

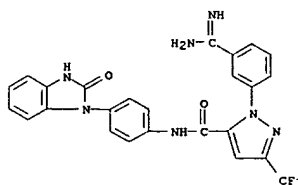
CM 1

CRN 774218-59-6

CMF C25 H18 F3 N7 O2

L23 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)



CM 2

CRN 76-05-1

CMF C2 H F3 O2



IT

774218-59-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(pyrazole compounds, preparation, crystal structure, and dual inhibition of factors IXa and Xa)

of

RN

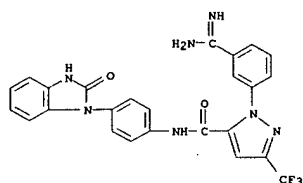
774218-59-6 CAPLUS

CN

1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)



IT 848393-47-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

of

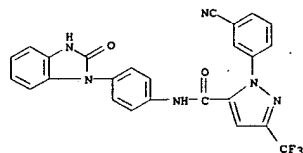
(pyrazole compounds, preparation, crystal structure, and dual inhibition of factors IXa and Xa)

RN

848393-47-5 CAPLUS

CN

1H-Pyrazole-5-carboxamide, 1-(3-cyanophenyl)-N-[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

15

THIS

THERE ARE 15 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2004:153586 CAPLUS

DOCUMENT NUMBER:

140:368084

TITLE:

1-(2-Naphthyl)-1H-pyrazole-5-carboxylamides as potent factor Xa inhibitors. Part 2: A survey of P4 motifs
Jia, Zhaozhong J.; Wu, Yanhong; Huang, Wenrong;

AUTHOR(S):

Zhang,

Penglie; Clizbe, Lane A.; Goldman, Erick A.; Sinha, Uma; Arfsten, Ann E.; Edwards, Susan T.; Alphonso, Marilyn; Hutchaleelaha, Athiwat; Scarborough, Robert M.; Zhu, Bing-Yan
Millennium Pharmaceuticals, Inc., South San Francisco,

CORPORATE SOURCE:

CA, 94080, USA

SOURCE:

Bioorganic & Medicinal Chemistry Letters (2004),
14(5), 1221-1227

PUBLISHER:

CODEN: BMCLE8; ISSN: 0960-894X

DOCUMENT TYPE:

Elsevier Science B.V.

LANGUAGE:

Journal

AB

A variety of P4 motifs have been examined to increase the binding

affinity

and in vitro anticoagulant potency of our biphenyl 1-(2-naphthyl)-1H-pyrazole-5-carboxylamide-based IXa inhibitors. Highly potent 2-naphthyl-P1 IXa inhibitors (K_i52 nM) with improved in vitro anticoagulant activity (2-TGS1 μM) and respectable pharmacokinetic properties have been discovered.

IT

684233-39-4 684233-40-7 684233-41-8

684233-42-9 684233-66-7 684233-70-3

684233-71-4 684233-72-5 684233-73-6

684233-74-7 684233-75-8

RL: PAC (Pharmacological activity); BIOL (Biological study)

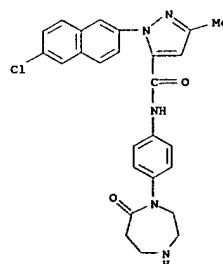
(1-(2-Naphthyl)-1H-pyrazole-5-carboxylamides as potent factor Xa inhibitors)

RN

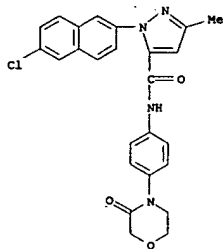
684233-39-4 CAPLUS

CN

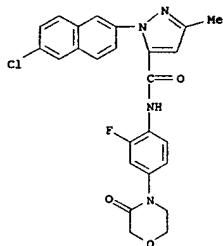
1H-Pyrazole-5-carboxamide, 1-(6-chloro-2-naphthalenyl)-N-[4-(hexahydro-7-oxo-1H-1,4-diazepin-1-yl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)



L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 RN 684233-40-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-(6-chloro-2-naphthalenyl)-3-methyl-N-[4-(3-oxo-4-morpholinyl)phenyl]- (9CI) (CA INDEX NAME)

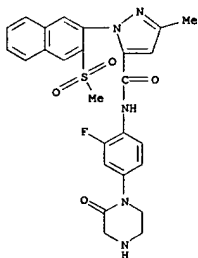


RN 684233-41-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-(6-chloro-2-naphthalenyl)-N-[2-fluoro-4-(3-oxo-4-morpholinyl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)

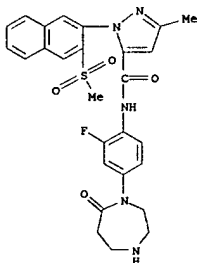


RN 684233-42-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-(6-chloro-2-naphthalenyl)-3-methyl-N-[4-(2-oxo-1-piperidinyl)phenyl]- (9CI) (CA INDEX NAME)

L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

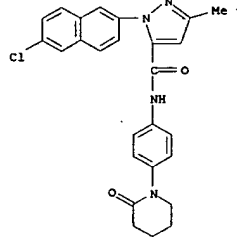


RN 684233-71-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(hexahydro-7-oxo-1H-1,4-diazepin-1-yl)phenyl]-3-methyl-1-[3-(methylsulfonyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

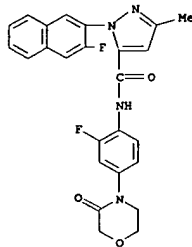


RN 684233-72-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(tetrahydro-5-oxo-1,4-oxazepin-4(5H)-yl)phenyl]-3-methyl-1-[3-(methylsulfonyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

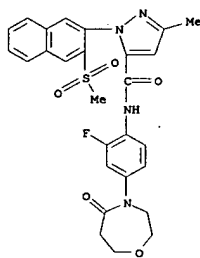


RN 684233-66-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-(3-fluoro-2-naphthalenyl)-N-[2-fluoro-4-(3-oxo-4-morpholinyl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)

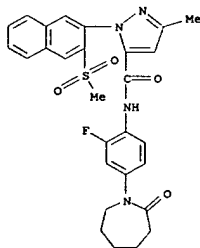


RN 684233-70-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(2-oxo-1-piperazinyl)phenyl]-3-methyl-1-[3-(methylsulfonyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

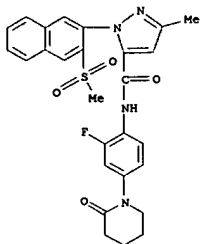


RN 684233-73-6 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(hexahydro-2-oxo-1H-azepin-1-yl)phenyl]-3-methyl-1-[3-(methylsulfonyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

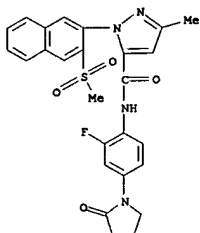


RN 684233-74-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(2-oxo-1-piperidinyl)phenyl]-3-methyl-1-[3-(methylsulfonyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 684233-75-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(2-oxo-1-pyrrolidinyl)phenyl]-3-methyl-1-[3-(methylsulfonyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)



IT 684233-69-0
 RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); BIOL (Biological study)
 (1-(2-Naphthyl)-1H-pyrazole-5-carboxylamides as potent factor Xa inhibitors)
 RN 684233-69-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[2-fluoro-4-(3-oxo-4-morpholinyl)phenyl]-3-methyl-1-[3-(methylsulfonyl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

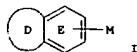
L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:725629 CAPLUS
 DOCUMENT NUMBER: 133:296430
 TITLE: Preparation of aryl sulfonyls as factor Xa inhibitors
 INVENTOR(S): Wexler, Ruth R.; Jacobson, Irina C.
 PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
 SOURCE: PCT Int. Appl., 116 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000059902	A2	20001012	WO 2000-US8364	20000330
WO 2000059902	A3	20010426		
W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, FL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2368630	A1	20001012	CA 2000-2368630	20000330
EP 1175419	A2	20020130	EP 2000-923096	20000330
EP 1175419	B1	20030528		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 241621	T	20030615	AT 2000-923096	20000330
ES 2197092	T3	20040101	ES 2000-923096	20000330
US 6399644	B1	20020604	US 2000-540467	20000331
US 2003050315	A1	20030313	US 2002-74301	20020212
US 6689770	B2	20040210		

PRIORITY APPLN. INFO.:
 US 1999-127634P P 19990402
 WO 2000-US8364 W 20000330
 US 2000-540467 A3 20000331

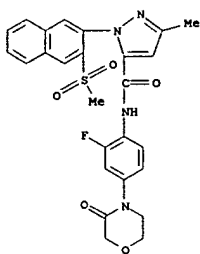
OTHER SOURCE(S): MARPAT 133:296430
 GI



AB Aryl sulfonyls I [ring D is absent or is CH2N:CH, CH:NCH2, aromatic system containing heteroatoms, etc.; E = Ph, pyridyl, pyrazinyl, etc.; M = heterocyclyl], effective factor Xa inhibitors (no data), were prepared. E.g., N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-1-(4-methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide was prepared.
 IT 300710-13-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT

10519356a.trn

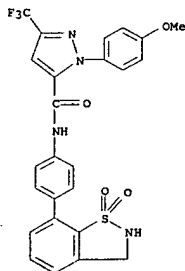
L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

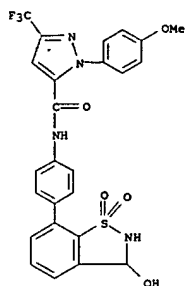
L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

(Reactant or reagent); USES (Uses)
 (prepn. of aryl sulfonyls as factor Xa inhibitors)
 RN 300710-13-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-1-(4-methoxyphenyl)-3-(trifluoromethyl)- (9CI)
 (CA INDEX NAME)

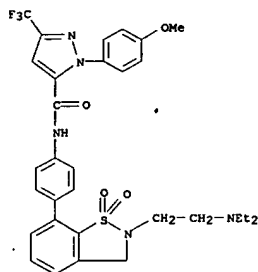


IT 300710-14-9P 300710-15-0P 300710-16-1P
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 300710-23-0P 300710-24-1P 300710-25-2P
 300710-26-3P 300710-27-4P 300710-28-5P
 300710-29-6P 300710-30-9P 300710-31-0P
 300710-32-1P 300710-33-2P 300710-34-3P
 300710-35-4P 300710-36-5P 300710-37-6P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of aryl sulfonyls as factor Xa inhibitors)
 RN 300710-14-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[4-(2,3-dihydro-3-hydroxy-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-1-(4-methoxyphenyl)-3-(trifluoromethyl)- (9CI)
 (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

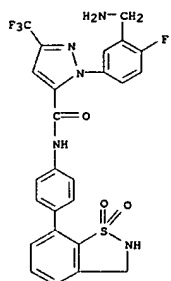


RN 300710-15-0 CAPLUS
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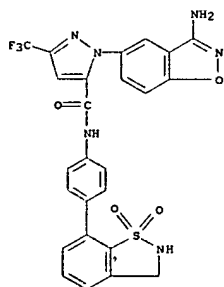


RN 300710-16-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

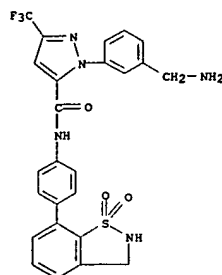


RN 300710-19-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-amino-1,2-benzisoxazol-5-yl]-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

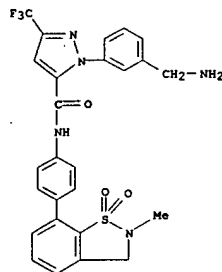


RN 300710-20-7 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[4-[2-(cyanomethyl)-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-1-(4-methoxyphenyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

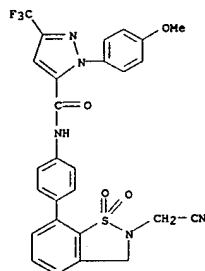


RN 300710-17-2 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

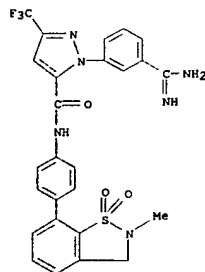


RN 300710-18-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)-4-fluorophenyl]-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

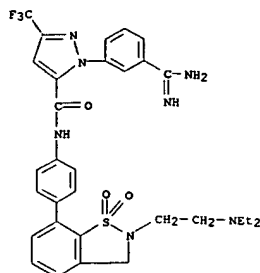


RN 300710-21-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

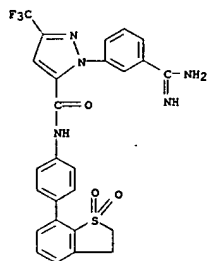


RN 300710-22-9 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-[2-(2-diethylamino)ethyl]-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

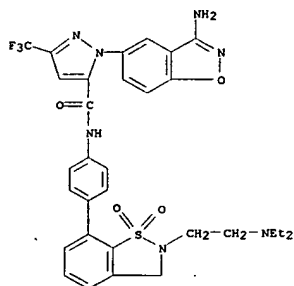


RN 300710-23-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-(aminomethyl)phenyl)-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

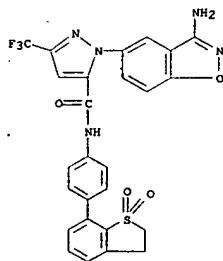


RN 300710-24-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-(aminomethyl)phenyl)-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

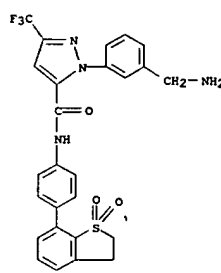


RN 300710-27-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

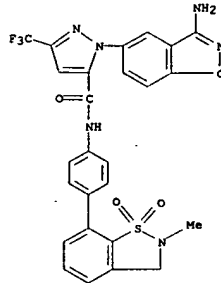


RN 300710-28-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-(aminomethyl)phenyl)-N-[4-(2-(diethylamino)ethyl)-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

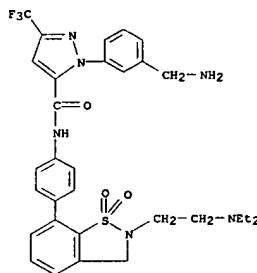


RN 300710-25-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

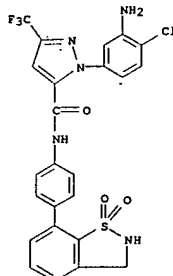


RN 300710-26-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-1,2-benzisoxazol-5-yl)-N-[4-(2-(diethylamino)ethyl)-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

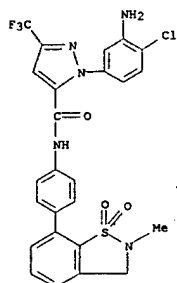


RN 300710-29-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-4-chlorophenyl)-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

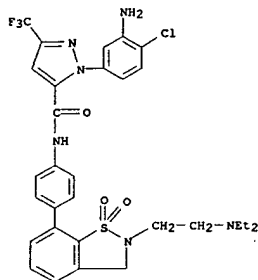


RN 300710-30-9 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-4-chlorophenyl)-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

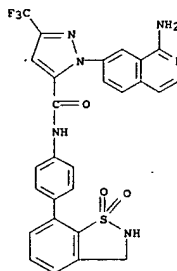


RN 300710-31-0 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-4-chlorophenyl)-N-[4-{2-(diethylamino)ethyl}-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

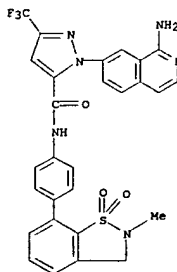


RN 300710-32-1 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(3-amino-4-chlorophenyl)-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



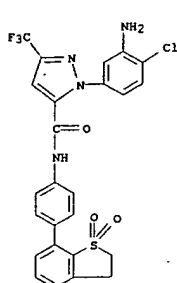
RN 300710-35-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(1-amino-7-isoquinolinyl)-N-[4-(2,3-dihydro-2-methyl-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



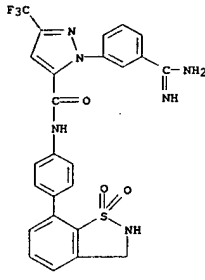
RN 300710-36-5 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(1-amino-7-isoquinolinyl)-N-[4-{2-(diethylamino)ethyl}-2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl]phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10519356a.trn

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

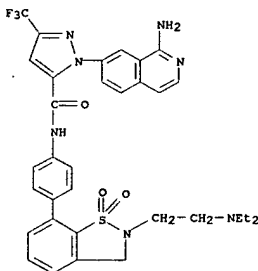


RN 300710-33-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

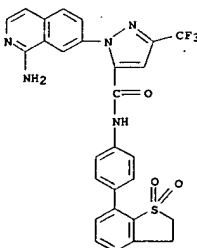


RN 300710-34-3 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(1-amino-7-isoquinolinyl)-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



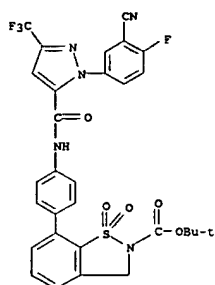
RN 300710-37-6 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-(1-amino-7-isoquinolinyl)-N-[4-(2,3-dihydro-1,1-dioxido-1,2-benzisothiazol-7-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



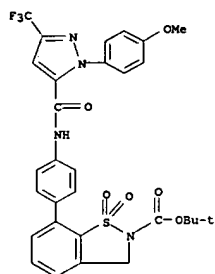
IT 300710-47-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aryl sulfonyls as factor Xa inhibitors)

RN 300710-47-8 CAPLUS
CN 1,2-Benzisothiazole-2(3H)-carboxylic acid, 7-[4-[[[1-(3-cyano-4-fluorophenyl)-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-, 1,1-dimethylethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



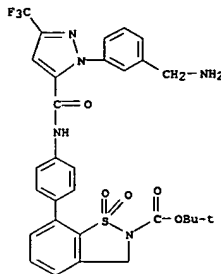
IT 300710-44-5P 300710-45-6P 300710-46-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of aryl sulfonyls as factor Xa inhibitors)
 RN 300710-44-5 CAPLUS
 CN 1,2-Benzisothiazole-2(3H)-carboxylic acid, 7-[4-[[[1-(4-methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-, 1,1-dimethylethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)



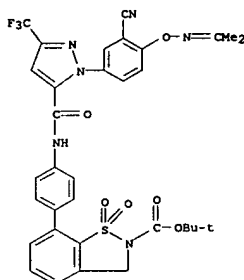
RN 300710-45-6 CAPLUS

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CN 1,2-Benzisothiazole-2(3H)-carboxylic acid, 7-[4-[[[1-(3-aminomethyl)phenyl)-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-, 1,1-dimethylethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)



RN 300710-46-7 CAPLUS
 CN 1,2-Benzisothiazole-2(3H)-carboxylic acid, 7-[4-[[[1-(3-cyano-4-[[[1-methylethylidene)amino]oxy]phenyl]-3-(trifluoromethyl)-1H-pyrazol-5-yl]carbonyl]amino]phenyl]-, 1,1-dimethylethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)



L23 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:83115 CAPLUS
 DOCUMENT NUMBER: 132:137392
 TITLE: Preparation of azoles as Factor Xa inhibitors.
 INVENTOR(S): Pinto, Donald Joseph Phillip; Pruitt, James Russell;
 Cacciola, Joseph; Fevig, John Matthew; Han, Qi;
 Orwat,
 Michael James; Quan, Mimi Lifan; Rossi, Karen Anita
 PATENT ASSIGNEE(S): Dupont Pharmaceuticals Co., USA
 SOURCE: U.S., 152 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6020357	A	20000201	US 1997-995834	19971222
US 6548512	B1	20030415	US 2000-492708	20000127
PRIORITY APPLN. INFO.:				P 19961223
				F 19970620
				A3 19971222

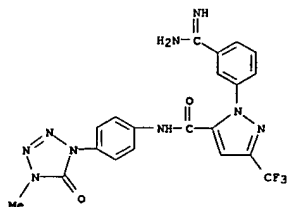
OTHER SOURCE(S): MARPAT 132:137392

GI

DEG(CH₂)_n ZAB I

AB Title compds. [I; ring M contains, in addition to J, 0-3 N atoms; J = N, NH;
 D = CN, C(:NR8)NR7R9, C(O)NR7R8, etc.; E = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; DEG = R-substituted pyridyl; R = H, halo, CF₃, etc.; G = absent, NHCH₂, OCH₂, etc.; Z = C1-4 alkylene, (CH₂)₂O(CH₂)₂, etc.; R1a, R1b = absent, NMe, OMe, etc.; A = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S; B = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S, etc.; R7 = H, OH, C1-6 alkyl, etc.; R8, R9 = H, C1-6 alkyl, (CH₂)_nPh;
 n = 0-3; r = 0-3; s = 0-2; with proviso], useful as inhibitors of factor Xa, were prepared and formulated. Thus, treatment of 4-(o-tert-BUSO₂)phenyl]aniline with Me₃Al/hexane in CH₂Cl₂ followed by the addition of Me 1-(3-cyanophenyl)imidazol-2-ylcarboxylate (preparation described), and the Pinner reaction of the resulting intermediate afforded 1-(3-aminophenyl)-2-[(2'-aminosulfonyl-1,1'-biphen-4-yl)aminocarbonyl]imidazole. Several I showed KI ≤10 μM against

L23 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 Factor Xa and thrombin.
 IT 209956-77-4P 209956-78-5P 209958-09-8P
 209958-10-1P
 RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of azoles as Factor Xa inhibitors)
 RN 209956-77-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4,5-
 dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-
 (9CI) (CA INDEX NAME)



RN 209956-78-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminoiminomethyl)phenyl]-N-[4-(4,5-
 dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-,
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

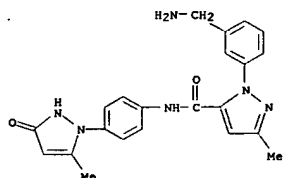
CH 1

CRN 209956-77-4
 CMF C20 H16 F3 N9 O2

L23 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 (9CI) (CA INDEX NAME)

CH 1

CRN 209958-09-8
 CMF C22 H22 N6 O2



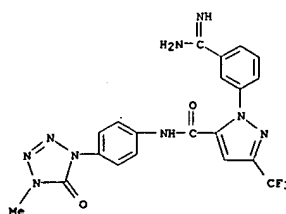
CH 2

CRN 76-05-1
 CMF C2 H F3 O2



IT 209959-74-0P 209960-49-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of azoles as Factor Xa inhibitors)
 RN 209959-74-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 1-(3-cyanophenyl)-N-[4-(4,5-dihydro-4-methyl-5-
 oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

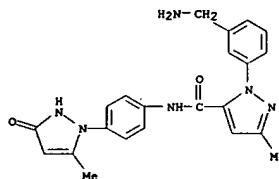


CH 2

CRN 76-05-1
 CMF C2 H F3 O2

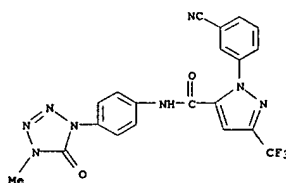


RN 209958-09-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-5-
 methyl-3-oxo-1H-pyrazol-1-yl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)

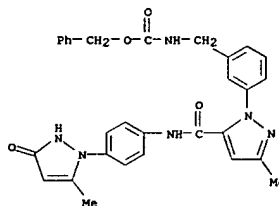


RN 209958-10-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-5-
 methyl-3-oxo-1H-pyrazol-1-yl)phenyl]-3-methyl-, mono(trifluoroacetate)

L23 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209960-49-6 CAPLUS
 CN Carbamic acid, [[3-[5-[[[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-
 yl)phenyl]amino]carbonyl]-3-methyl-1H-pyrazol-1-yl]phenyl]methyl]-,
 phenylmethyl ester (9CI) (CA INDEX NAME)



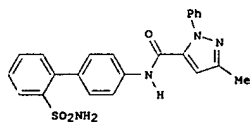
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L23 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1999:9820 CAPLUS
 DOCUMENT NUMBER: 130:81510
 TITLE: Preparation of phenylpyrazolecarboxamides as
 coagulation factor Xa inhibitors
 INVENTOR(S): Galemmo, Robert Anthony, Jr.; Dominguez, Celis;
 Fevig,
 John Matthew; Han, Qi; Lam, Patrick Yuk-sun; Pinto,
 Donald Joseph Philip; Pruitt, James Russell; Quan,
 Mimi Lifan
 PATENT ASSIGNEE(S): The Du Pont Merck Pharmaceutical Company, USA
 SOURCE: PCT Int. Appl., 239 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9857937	A2	19981223	WO 1998-US12681	19980618
WO 9857937	A3	19990318		
W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
ZA 9805251	A	19991217	ZA 1998-5251	19980617
CA 2290982	A1	19981223	CA 1998-2290982	19980618
AU 9881503	A	19990104	AU 1998-81503	19980618
US 5998424	A	19991207	US 1998-99752	19980618
EP 991625	A2	20000412	EP 1998-931355	19980618
EP 991625	B1	20050601		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
BR 9810151	A	20000808	BR 1998-10151	19980618
EE 9900584	A	20000815	EE 1999-584	19980618
SI 20208	A	20001031	SI 1998-20043	19980618
HU 200003906	A2	20010528	HU 2000-3906	19980618
JP 2002507968	T	20020312	JP 1999-504786	19980618
AT 296805	T	20050615	AT 1998-931355	19980618
ES 2239806	T3	20051001	ES 1998-931355	19980618
PT 991625	T	20051031	PT 1998-931355	19980618
US 6403620	B1	20020611	US 1999-393782	19990910
LV 12516	B	20010320	LV 1999-177	19991216
NO 9906316	A	19991217	NO 1999-6316	19991217
LT 4702	B	20000925	LT 1999-146	19991217
WO 2001080762	A2	20011101	WO 2001-US13280	20010424
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CF, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN,				

L23 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 US 2001-757385 A1 20010108
 WO 2001-US13280 A2 20010424
 US 2001-40269 A1 20011029
 US 2002-99187 A1 20020313
 US 2002-139153 A2 20020502
 US 2002-262516 A2 20020930

OTHER SOURCE(S): MARPAT 130:81510
 GI

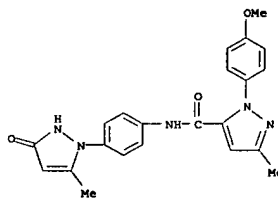


II

AB EZ1M [I; E = halo, OH, alkyl, alkoxy, etc.; M = 22ZAB; A = (un)substituted carbocyclene, -heterocyclene; B = H, Y, XY; X = alkylene, CO, O, (un)substituted NH, etc.; Y = amino(alkyl), substituted carbocyclyl, -heterocyclyl, etc.; Z = bond, (heteroatom- or functional group-interrupted) alkylene, etc.; Z1 = (un)substituted Ph, Z2 = N-containing heteroarylene, etc.] were prepared. Thus, MeCOCH2C(=NOMe)CO2Et was cyclocondensed with PhNHNH2 and the product amidated by 4-(H2N)C6H4C6H4(SO2NHMe3)-2 to give, after deprotection, title compound II.
 IT Data for biol. activity of I were given.
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (Preparation of phenylpyrazolecarboxamides as coagulation factor Xa inhibitors)
 RN 218630-82-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, N-[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-yl)phenyl]-1-(4-methoxyphenyl)-3-methyl- (5CI) (CA INDEX NAME)

L23 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 GW, ML, MR, NE, SN, TD, TG
 US 2002106604 A1 20020808 US 2001-40269 20011029
 US 6705863 B2 20040316 US 2002-150698 20020516
 US 2003092740 A1 20030515 US 2003-632482 20030801
 US 6602895 B2 20030805 US 2003-660857 20030912
 US 7059850 B1 20060613 US 2003-718779 20031120
 US 2004048223 A1 20040311 US 2004-799432 20040312
 US 7125248 B2 20061024 US 2004-341318 20041125
 US 2004110110 A1 20040610 US 1997-50219P P 19970619
 US 7134874 B2 20061114 US 1997-878885 A 19970619
 US 2004209218 A1 20041021 US 1998-76691P P 19980227
 US 7121825 B2 20061017 US 1997-50342P P 19970620
 JP 2005118592 A 20050512 US 1997-947080 A2 19971008
 PRIORITY APPLN. INFO.: US 1998-99752 A3 19980618
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L23 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

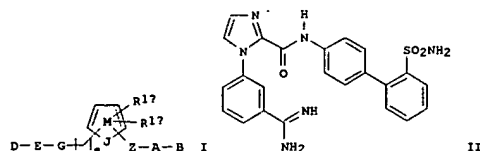


L23 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1998:479506 CAPLUS
 DOCUMENT NUMBER: 129:109090
 TITLE: Preparation of nitrogen-containing heteroaromatics as factor Xa inhibitors
 INVENTOR(S): Pinto, Donald Joseph Phillip; Pruitt, James Russell; Cacciola, Joseph; Fevig, John Matthew; Han, Qi;
 ORwat,
 Michael James; Quan, Mimi Lifan; Rossi, Karen Anita
 PATENT ASSIGNEE(S): The Dupont Merck Pharmaceutical Co., USA
 SOURCE: PCT Int. Appl., 438 pp.
 CODEN: PIXXD2
 PATENT: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9828269	A1	19980702	WO 1997-US22895	19971215
W: AM, AU, AZ, BR, BY, CA, CN, CZ, EE, HU, IL, JP, KG, KR, KZ, LT, LV, MD, MK, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, UA, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2275796	A1	19980702	CA 1997-2275796	19971215
AU 9856020	A	19980717	AU 1998-56020	19971215
AU 730224	B2	20010301		
EP 946508	A1	19991006	EP 1997-952409	19971215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
EE 9900316	A	20000215	EE 1999-316	19971215
SI 20017	A	20000229	SI 1997-20082	19971215
CN 1246847	A	20000308	CN 1997-181852	19971215
BR 9714073	A	20000509	BR 1997-14073	19971215
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NO 313190	B1	20020826		
MX 9905878	A	20000131	MX 1999-5878	19990622
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LV 12430	B	20000720	LV 1999-99	19990730
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			US 1997-879944	A 19970620
			WO 1997-US22895	W 19971215

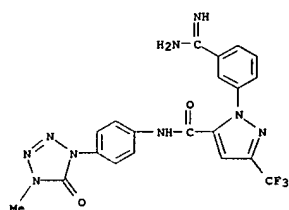
OTHER SOURCE(S): MARPAT 129:109090
 GI

L23 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB The title compds. [I: ring M contains, in addition to J, 0-3 N atoms; J = N, NH; D = CN, C(=NR8)NR7R9, C(O)NR7R8, etc.; E = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; DEG = R-substituted pyridyl; R = H, halo, CF3, etc.; G = absent, NHCH2, OCH2, etc.; Z = C1-4 alkylene, (CH2)rO(CH2)r, etc.; R1a, R1b = absent, NMe, OMe, etc.; A = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S; B = (un)substituted C3-10 carbocyclic residue, 5-10 membered heterocyclic containing from 1-4 heteroatoms selected from N, O, and S, etc.; R7 = H, OH, C1-6 alkyl, etc.; R8, R9 = H, C1-6 alkyl, (CH2)nPh; n = 0-3; r = 0-3; s = 0-2), useful as inhibitors of factor Xa, were prepared and formulated. Thus, treatment of 4-[o-(tert-BuSO2)phenyl]aniline with Me3Al/hexane in CH2Cl2 followed by the addition of Me 1-(3-cyanophenyl)imidazol-2-ylcarboxylate (preparation described), and the Pinner reaction of the resulting intermediate afforded the title compound II. A number of compds. I were found to exhibit a Ki of $\leq 10 \mu\text{M}$ against factor Xa. Some compds. I were evaluated and found to exhibit Ki of $< 10 \mu\text{M}$ against thrombin.
 IT 209956-77-4P 209956-78-5P 209958-09-8P
 209958-10-1P
 RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 [preparation of nitrogen-containing heteroaroms. as factor Xa inhibitors]
 RN 209956-77-4 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-(9CI)
 (CA INDEX NAME)

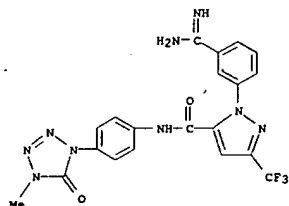
L23 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 209956-78-5 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(4,5-dihydro-4-methyl-5-oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209956-77-4
 CMF C20 H16 F3 N9 O2



CM 2

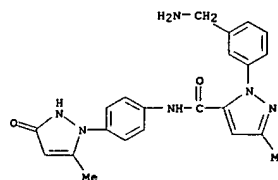
CRN 76-05-1
 CMF C2 H F3 O2



10519356a.trn

L23 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

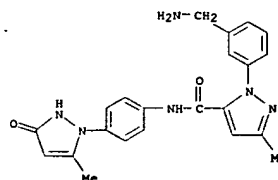
RN 209958-09-8 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-yl)phenyl]-3-methyl- (9CI) (CA INDEX NAME)



RN 209958-10-1 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 1-[3-(aminomethyl)phenyl]-N-[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-yl)phenyl]-3-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 209958-09-8
 CMF C22 H22 N6 O2



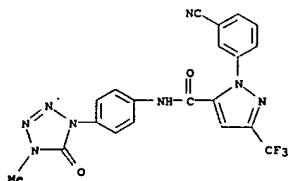
CM 2

CRN 76-05-1
 CMF C2 H F3 O2

L23 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

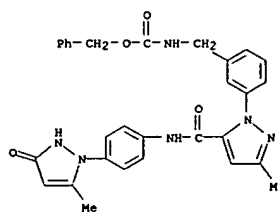


IT 209959-74-0P 209960-49-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of nitrogen-containing heteroaroms. as factor Xa
 inhibitors)
 RN 209959-74-0 CAPLUS
 CN 1H-Pyrazole-5-carboxamide,
 1-(3-cyanophenyl)-N-[4-(4,5-dihydro-4-methyl-5-
 oxo-1H-tetrazol-1-yl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 209960-49-6 CAPLUS
 CN Carbamic acid, [[3-[5-[[[4-(2,3-dihydro-5-methyl-3-oxo-1H-pyrazol-1-
 yl)phenyl]amino]carbonyl]-3-methyl-1H-pyrazol-1-yl]phenyl]methyl]-,
 phenylmethyl ester (9CI) (CA INDEX NAME)

L23 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR
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 FORMAT

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TOTAL

ENTRY

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FULL ESTIMATED COST

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

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CA SUBSCRIBER PRICE

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